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Computer Science Research Institute 2004 Annual Report of Activities

David E. Womble, Barbara J. DeLap, and Deanna R. Ceballos

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Abstract

This report summarizes the activities of the Computer Science Research Institute (CSRI) at Sandia National Laboratories during the period January 1, 2004 to December 31, 2004. During this period the CSRI hosted 166 visitors representing 81 universities, companies and laboratories. Of these 65 were summer students or faculty. The CSRI partially sponsored 2 workshops and also organized and was the primary host for 4 workshops. These 4 CSRI sponsored workshops had 140 participants--74 from universities, companies and laboratories, and 66 from Sandia. Finally, the CSRI sponsored 14 long-term collaborative research projects and 5 Sabbaticals.

Contents

Chapter 1. CSRI Overview

1.1. Introduction

The Computer Science Research Institute (CSRI) at Sandia National Laboratories brings together researchers from universities and the national laboratories to solve problems in computer science, computational science and mathematics and to provide new capabilities in modeling and simulation. Participants are also encouraged to develop long-term relationships with laboratory scientists and researchers.

Through the inclusion of university faculty, the CSRI expands the range of expertise and research capabilities that can be applied to problems in modeling and simulation at the national laboratories. Through the interactions with laboratory scientists, researchers from universities and industry are exposed to computational problems that arise at the laboratories in connection with their DOE stockpile stewardship mission.

The Computer Science Research Institute also includes both graduate and undergraduate student programs. These include post-doctoral positions, summer jobs and graduate fellowships. The CSRI encourages students to choose careers in computer science, computational science and mathematics that support directly the challenges of national security programs.

The Computer Science Research Institute complements existing laboratory research programs and university alliances. It provides both a physical and technical focal point for identifying problems, for conducting research and for developing and strengthening interactions between the university and laboratory researchers.

This report presents an overview of the CSRI and describes the projects, visitor programs, and other activities conducted by the CSRI during the period January 1, 2004 to December 31, 2004.

1.2. Technical Focus of the CSRI

A number of potential long-term focus areas for the Sandia program in FY04 are listed and described below. This list represents key technologies in the high-performance massively parallel computing area with the potential to provide substantial benefit in efficiency and accuracy for the Sandia engineering analysis codes and other codes used or being developed for stockpile stewardship applications. Indeed, in some cases the focus areas include breakthrough technology which, when developed, will enable entirely new classes of simulations to be performed. The focus areas are divided into a small number of overarching technical areas, specifically, Algorithms and Computational Mathematics, Enabling Technologies, and System Software.

1.2.1 Algorithms and Computational Mathematics Focus Area:

1.2.1.1 Design and Optimization: As the ability to do "forward" simulations increases, the ability to do the "inverse" problem needs to be developed, e.g., parameter identification and system design, as well as the traditional inverse problems of applied mathematics. Optimization tends to be very application-specific, although some toolkits have been developed that can be generally applied. Current research efforts include work on large-scale optimization, global optimization, and discrete optimization.

1.2.1.2 Linear Solvers: Linear solvers are at the heart of many engineering simulations. There are many algorithms available; however, significant challenges remain. These challenges include the development of scalable preconditioners and preconditioners designed for the specific needs of various applications. Much attention is currently focused on "multiscale" methods and preconditioners as the hope for truly scalable solvers, but a lot of work remains to be done, especially for unstructured adaptive grids, systems of equations, and complex boundary conditions. Additional work is also needed in many other related areas, including algebraic preconditioners, coupling direct methods for better or more robust convergence, ways to improve performance for machines with deep memory hierarchies, and developing solvers for matrices without the traditional finite-element structure, e.g., in circuit simulation.

1.2.1.3 Nonlinear Solvers: Nonlinear solvers often depend on repeated linear solvers, but there are additional research questions. For example, it will be necessary to solve systems with hundreds of variables for 3-D high-fidelity simulations. Present technology is expected to achieve tens of variables within the next year, falling far short of the ultimate requirement. Newton methods and their use in conjunction with preconditioned Krylov methods for specific problems, are of particular interest.

1.2.1.4 Eigensolvers: Many scientific and engineering problems require the eigenvalues and eigenvectors of extremely large matrices. Examples of particular interest include modal analysis for structural dynamics, minimum energy eigenfunction calculations in quantum chemistry models, and detecting the onset of turbulence in fluid flow. A common feature of these eigenvalue problems is that the number of eigenvalues required is small relative to the size of the matrices, the matrix systems are often very sparse, and only the action of the matrix on a vector (or several of them) is available. Standard techniques that involve directly factoring the matrix (including sparse direct methods) are often impractical for these problems because of excessive memory and computational requirements. Algorithmic work is needed on scalable eigensolvers, reduced accuracy algorithms, parallel implementations and application-focused algorithmic research.

1.2.1.5 Algorithms for Differential and Integral Equations: Differential or integral equations lie at the heart of most engineering simulations. A mathematical analysis of these equations can often reduce the amount of computing needed by simplifying or improving models, choosing better algorithms, or designing better computational experiments. Research topics of interest include coupling or de-coupling of scales, subgrid modeling, asymptotics, bifurcation, and stability analysis.

1.2.1.6 Complex Phenomena: This is a very large area, but general goals include identifying and quantifying the effects of uncertainty, developing a predictive capability for complex systems and processes based on computational "experiments," and algorithms that reduce fundamental computational complexity. Topics of interest include stochastic finite elements, sensitivity analysis, experimental design, stability analysis, summability methods, and general methods for handling multiscale (time and space) phenomena.

1.2.1.7 Adaptivity: The purpose of the adaptivity area is to develop the methodologies and algorithms for finite element error estimation and adaptive computing, with the general goal being to reduce the cost of computing by increasing the mesh resolution only in areas where needed. Finite element error estimation addresses the discretization error of the finite element solution for some (local) quantity of interest. The goal is to obtain tight bounds or estimates of the error in a way that is relatively cheap to compute (compared to the cost of solving the original problem).

1.2.2 Enabling Technologies Focus Area:

1.2.2.1 Meshing: Meshing is a time consuming and difficult part of any engineering simulation, yet the quality of the simulation is highly dependent on the quality of the mesh. Of particular interest are hexahedral meshes and high-quality hex-tet meshes. Research questions here include mesh

connectivity, mesh optimization, and mesh refinement. Fully automatic methods and the ability to mesh large complex geometries are of particular interest. The general issue of a robust parallel meshing toolkit remains a high-priority goal of the high-performance computing (HPC) programs at the laboratories.

1.2.2.2 Automatic Mesh Refinement and Dynamic Load Balancing: More and more simulation codes include the ability to handle multiple meshes or to automatically refine meshes, and the efficient parallel implementation of these codes will require dynamic load balancing algorithms. Much of the current work is on design and implementation, but as the implementations become available, many new research questions will be raised. The need for dynamic load balancing will be more acute in heterogeneous environments such as will be developed under DisCom2. There will also be the need for "online" load balancing algorithms.

1.2.2.3 Visualization: The visualization needs at Sandia have outstripped the abilities of the commercially available tools. New algorithms are needed, and there are many questions to be answered about the appropriate and optimal visualization algorithms that should be used for SSP applications. Also, there is the question of where and when to do the visualization in a large simulation, e.g., as a post-processing operation or as a runtime process, on a stand-alone platform or on the MP machine directly, etc. The answer to these questions will have a major impact on the type of algorithms that are developed for visualization applications. Emphasis in this area will be on scalable visualization tools and algorithms for very large data sets. Distributed, commodity visualization platforms are being developed as an alternative to the costly, nonscalable platforms currently available.

1.2.3 System Software Focus Area:

1.2.3.1 Operating Systems: The operating system is a critical component in the effective and efficient use of massively parallel processing (MPP) computers. Current research topics include the use of commodity operating systems (primarily Linux) with modifications and extensions for MPP computers and distributed, cluster-based, virtual MPP computers. As in other areas, a key focus is on scalability. Projects include adding simple memory management and process management to Linux to improve performance while preserving Linux's portability and expandability, improving communication and connectivity, and fault tolerance. The efficient use of SMP nodes within the MPP computing environment is also being considered; this includes the development and implementation of efficient thread and virtual node capabilities and the efficient utilization of resources that are un-partitionable, such as the network interface.

1.2.3.2 Environments: An effective environment must address several issues. First, it must provide a fast and "user friendly" environment that allows designers to access easily all of the modeling tools, the data comprehension tools, the problem setup tools and the resources required. Second, it must provide a robust and efficient environment for developers to prototype new methods, algorithms and physics, without redoing major portions of the existing codes. Examples exist of application problem-solving-environments aimed at designers, but these are all "one-of-a-kind" products that are developed for a specific physics code. Examples also exist of component interfaces that allow specific methods to be rapidly prototyped, but again these are not general-purpose, nor are they in common use. Finally, new software tools are needed to model and predict the performance of code and algorithms on MPP computers. The development of tools that combine object-based, Web-centric, client-server technology with high-performance parallel server technology, made available on demand, will also be pursued.

1.2.3.3 I/O: Large-scale, simulation-based analysis requires efficient transfer of data among simulation, visualization, and data management applications. Current efforts seek to improve I/O performance of parallel codes by facilitating I/O operations from multiple nodes in parallel through highly portable user-level programming interfaces. This work will involve design, implementation, and testing of a portable parallel file system. Ideally, the parallel file system should include a server

side, which may require a particular hardware configuration, and a client side, which is appropriate for use on any ASCI platform. This is not a replacement for MPI-IO. Just as the MPI data movement standard relies on an underlying message-passing or remote memory access protocol, the MPI-IO standard relies on an underlying file system. The goal is to produce at least a prototype of such a system and, if possible, a product that is appropriate for any future (or current) machine.

1.2.3.4 Heterogeneous and Distributed Systems: Parallel computers based on heterogeneous clusters of commodity workstations are starting to appear and will become common. Yet the effective use of these machines presents many research problems. For example, resources such as processors must be scheduled and managed, systems must be fault-tolerant, operating systems must be compatible, protocols for communication must be established, environments must be developed, and the integrated system must be latency-tolerant. The distinguishing feature for work in this area will be scalability to terascale and larger distributed systems.

1.2.3.5 Architecture: Our basic architecture is influenced by the highly successful ASCI Red. Cplant™ follows this architecture in spirit if not in details. This project will consider new architectures that will scale to 100 TF, petaflops, and beyond. Among other things is the need for research into interconnect technologies (hardware and software). In addition, for many current and future supercomputing applications, the enormity of the data in processing or post-processing for visualization is a major consideration. This project will consider such questions as how this should affect the architecture of future machines.

1.3. Research opportunities at the CSRI

The CSRI presents many opportunities for collaborations between university researchers and laboratory scientists in the areas of computer science, computational science and mathematics. These include the following

1.3.1 Collaborative research projects. The CSRI accepts proposals for collaborative research projects lasting from one to three years. Projects must have a principle investigator and a Sandia collaborator. Projects should address one of the technical areas listed above and the work must be performed on-site at Sandia. Proposals may be submitted to the CSRI director at any time and must be approved by the CSRI executive board.

1.3.2 Postdoctoral appointments. The CSRI offers several postdoctoral positions each year. Postdoctoral positions are for one year and are renewable for one additional year. Applications should include a statement of research interests, a resume, and a list of references.

1.3.3 Summer faculty positions and long-term research visits. Faculty are invited to consider the CSRI for summer employment or for extended visits. Salaries are generally commensurate with academic year salaries. Proposals to hire research groups including both faculty and graduate students for the summer are also encouraged.

1.3.4 Faculty sabbaticals. Faculty may spend all or part of a sabbatical year at the CSRI. Proposals for sabbatical visits are accepted at any time and the salary depends on the normal academic year salary and the sabbatical salary.

1.3.5 Summer student positions. Students are encouraged to apply for summer positions at the CSRI. Employment is generally for eight to twelve weeks. Students may be associated with a research group (see Summer Faculty Positions above) or may apply independently.

1.3.6 Graduate Fellowships. The CSRI sponsors graduate fellowships through the Krell Institute and the National Physical Sciences Consortium (NPSC). For more information, students can contact the Krell Institute or the NPSC directly, or they may contact the CSRI.

1.3.7 Short term visits. The CSRI hosts approximately 100 research visits lasting from several days to weeks. The CSRI generally reimburses visitors for travel expenses.

1.3.8 Workshops. The CSRI hosts one to five workshops per year. Workshops are generally co-organized by Sandia staff and university researchers. Workshop proposals are accepted at any time.

Chapter 2. Research Projects

This chapter summarizes the major projects funded by the Computer Science Research Institute. Project proposals can be submitted to the CSRI at any time and are considered for funding by the Executive Board. Criteria for funding projects include technical excellence and quality of the work, impact on the ASCI program, and the strength and breadth of collaborations with Sandia technical staff. Generally these projects are intended to develop new collaborations with university researchers. Also, the work described in these proposals is performed on-site at Sandia National Laboratories, which improves both the strength and breadth of the collaborations. This distinguishes these projects (and the CSRI) from the normal contracting process at Sandia National Laboratories. The projects are listed in alphabetical order by the PI.

1) EMU code for shape optimization
   Dr. Florin Bobaru, University of Nebraska-Lincoln

2) Efficient Implementation for Overlapping File Access in MPI-IO
   Alok Choudhary, ECE Department, Northwestern University
   Wei-keng Liao, ECE Department, Northwestern University
   Kenin Coloma, Northwestern University

3) Surrogate-Based Optimization
   John E. Dennis, Jr., Rice University

4) Global-Basis method for fluid problems
   Professor Jacob Fish, Rensselaer Polytechnic Institute
   Haim Waisman, Ph.D. Student, Rensselaer Polytechnic Institute

5) Large-Scale PDE-Constrained Optimization
   Omar Ghattas, Carnegie Mellon University
   Lorenz Biegler, Carnegie Mellon University

6) Harvey Greenberg, University of Colorado at Denver

7) Research in Finite Element Simulations
   Max D. Gunzburger, Florida State University

8) Multiscale Methods in Science and Engineering
   Dr. Thomas J. R. Hughes, The Texas Institute of Computational and Applied Mathematics, The University of Texas at Austin

9) CSRI Executive Board Member
   Deepak Kapur, University of New Mexico

10) Understanding Performance of New PIM-Based Execution Models
    Peter M. Kogge, University of Notre Dame

11) Large Scale Eigenvalue Methods and Model Reduction of Second Order Systems
    Dan C. Sorensen, Rice University

12) Optimization Under Uncertainty
    John Renaud, University of Notre Dame

13) The Red Summit Project: Petaflops Scale Computing through Processor in Memory Architecture
Dr. Thomas Sterling, California Institute of Technology (Caltech)

14) Developing Pattern Search Methods for Constrained Optimization
Virginia Torczon, College of William and Mary
Robert Michael Lewis, College of William and Mary

Title: EMU code for shape optimization

PI: Dr. Florin Bobaru, University of Nebraska-Lincoln

Dates: May 9, 2004 – July 30, 2004

CSRI POC: Stewart Silling, (505) 844-3973

Project Summary:

My research interests are in the general area of computational mechanics. More specifically, I am interested in developing numerical algorithms for optimization of materials and structures. I have recently shown the benefits one can obtain in shape optimization of elastic and thermoelastic bodies if, instead of the classical Finite Element Method, a meshfree approach is used. I am interested in new algorithms that would push the current limits in optimal design of materials and structures. Combining shape and material optimization, or shape and topology optimization are issues I am currently considering. With powerful algorithms for optimization, one would expect breakthroughs in designing individual components of complex systems ranging from new paradigms for MEMS design to improved designs of large scale systems such as better thermal protective shields for space shuttle or damage tolerant armors. Nature has been perfecting and evolving systems of higher and higher complexity to adjust to challenging environments. My goals are to find algorithms that would use the fundamental minimum principles of mechanics and physics to produce designs of comparable efficiency and versatility as nature's answers to complex environments.

Research Proposal: This project plans to advance the methods of shape design sensitivity analysis to problems involving regular boundaries subject to singular transformations, and singular boundaries under regular or singular transformations (see Figure 1). The peridynamic theory developed by Dr. S.A. Silling of Sandia will be the analysis tool instead of the classical theory of elasticity.

The boundaries to be considered are either interior boundaries (that may represent cracks, material interfaces, phase changes, etc.) or outer boundaries. Due to this generality of the formulation, the same framework can be used to treat shape optimization problems as well as material optimization of two or multi-species composites (searching for the best shape of inclusions in an elementary volume element by varying the interface).

The problem of calculating sensitivities of a response functional to singular transformations of the boundary (inner or outer, regular or singular) of a body subject to mechanical loading has not been studied so far due to intrinsic difficulties of treating singular boundaries and discontinuous fields in formulations of boundary value problems. In particular, the classical formulation of linear fracture mechanics gives rise to the well-known square-root singularity of the stress field. Clearly, sensitivities of singular boundary (the crack for example) shape variations cannot be addressed in the classical setting.

The problem of calculating sensitivities of a response functional to singular transformations of the boundary (inner or outer, regular or singular) of a body subject to mechanical loading has not been studied so far due to intrinsic difficulties of treating singular boundaries and discontinuous fields in formulations of boundary value problems. In particular, the classical formulation of linear fracture mechanics gives rise to the well-known square-root singularity of the stress field. Clearly, sensitivities of singular boundary (the crack for example) shape variations cannot be addressed in the classical setting.

The peridynamic formulation in elasticity eliminates the difficulties of the classical continuum theories when dealing with spatial derivatives of discontinuous fields. In this formulation, long-range forces are represented by a pairwise force function with compact support acting between two nodes of the discretization. Cusp-like profiles are obtained for the opening of a crack and infinite stresses at the crack tip are eliminated. The ad-hoc assumptions that were proposed in the past to correct the unphysical infinite stresses from the classical linear fracture mechanics theory are now no longer needed. The same model is

used in the peridynamic formulation on and off the discontinuity present in the fractured elastic body. The meshfree character of the peridynamic theory makes it extremely suitable for numerical treatment of shape optimization problems based on sensitivities.

We propose to develop analytical and numerical sensitivities for singular transformations in elasticity using the peridynamic formulation. Based on these sensitivities it will be possible to develop shape optimization of elastic bodies with singular boundaries including bodies with cracks, notches, cusp-like shapes, etc. At the same time, material optimization of composite (searching for optimal shapes of inclusions) or Functionally Graded Materials (finding the optimal material gradation) will be possible since the boundaries in our formulation are both external and internal. Another possible application would be the sensitivity and uncertainty estimation for elastic bodies with large numbers of random cracks.

Collaborations: The current proposal is seeking collaboration with the author of the peridynamic theory, Sandia's Dr. Stewart A. Silling. Dr. Silling is also the primary developer of the EMU code that implements the peridynamic theory. Dr. Silling is strongly supporting the current proposal and has provided a supporting letter for a proposal submitted by the author of this proposal to the DOE Early Career PI Program. EMU is a meshfree method designed to model cracks, discontinuities, and other singularities that may exit in a body initially or emerge as a result of deformation. In addition, the EMU code is able to represent interfaces between materials by modifying the bond properties between the discretization points. Modeling complex heterogeneous materials is one of the areas in which the peridynamic theory seems to have a great potential. We propose to couple the sensitivity calculations for singular transformation to the EMU code and build an optimal design code based on the peridynamic formulation. Ideally, when completed, the peridynamic code and the new sensitivity formulations will interface and enhance the capabilities of the DAKOTA system developed at SANDIA.

Length of Participation and Location of visit
The proposed length of participation is for one-month summer faculty for three years at the Sandia National Laboratories, Albuquerque, NM. The starting date for our collaboration is 1st of August 2002. The visit during the 2002 summer will be focused on familiarization with the numerical implementation of the peridynamic theory, the EMU code. The basics ingredients of the sensitivity analysis with singular transformations for domains with singularities will be developed. For the remaining part of 2002 and before the summer of 2003, our collaboration will continue in various forms: Dr. Silling will be invited to present a seminar at the Department of Engineering Mechanics at University of Nebraska-Lincoln in the Fall of 2002. The author of the current proposal has a Master student who will be working to develop the computer programs for a proper coupling of the shape sensitivity analysis into Sandia's EMU code. Dr. Silling will be invited to participate in the graduate committee of the Master student.

The second visit (June 2003) will focus on the development of a series of optimization algorithms for shape and material optimization based on the developed sensitivity programs. We will test peridynamic formulation against some classical problems in shape optimization and, moreover, we will attempt solutions to singular problems never considered before. Parallel versions for the sensitivity calculations will be advanced.

The third visit (August 2004) will be dedicated to large-scale simulations involving hundreds and possibly thousands of design variables and the assessment of the benefits of the peridynamic formulation in optimal design of complex systems (complex geometries and complex material behavior). Problems of different scales will be considered. Comparisons with results provided by the DAKOTA system will be made.

Title: Efficient Implementation for Overlapping File Access in MPI-IO (Years Two and Three)

PI: Alok Choudhary, Northwestern University
Wei-keng Liao, Northwestern University

Dates: October 1, 2003 - August 15, 2004

CSRI POC: Eric Russell, (505) 844-3679

Project Summary:

Numerous studies of the I/O characteristics of parallel applications have shown that in most cases multiple processors access shared data objects. However, the partitioning and layout of the shared data objects to be stored in the memory can be different from its physical layout on disks, in which case the I/O performance can significantly degrade. In order to solve such problem, collective I/O was proposed in which each participated processor performs I/O on behalf of other processors and, then, all processors use available interconnection network to exchange the data so that each processor obtains the desired data. This technique has been adopted by MPI-IO, the I/O part of the MPI-2 standard, whose goal is to design a high-performance I/O library for parallel and distributed I/O. Collective I/O operations may have the situations that multiple processors issue concurrent read/write requests to overlapped regions in the shared file. The results of writing to the overlapped regions can be defined as written by one of the processors, an aggregation of all processors, or undefined. The mechanism of solving this problem, called atomicity, is implemented differently across file systems, which may involve locking shared files to guarantee the desired results. However, file locking reduces the parallelism of performing concurrent I/O and becomes the bottleneck of the collective operations. We propose to develop techniques to solve this problem. We plan to design a mechanism that automatically detects overlapping region accesses in the collective I/O operations in order to reduce the number of file locking, pass proper parameters to file locking mechanism, or even remove the locking.

ROMIO, a portable MPI-IO implementation, provides uniform parallel I/O APIs to access files on different file systems. Internally, ROMIO is built on top of ADIO, which is implemented separately on each file system using its native machine-dependent I/O library. When the underlying file system is the Network File System (NFS), ADIO use the file lock mechanism, `fcntl`, to perform non-coherent client-side caching on local processor memory by NFS default. This effect can prevent the file consistency problems occurred in other processors. ADIO disables client-side caching by locking the portion of the file being accessed so that the updated data can be flushed to the disk and viewable by other processors. This implementation results a pair of lock and unlock wraparound every native NFS read/write calls, even for those collective I/O performing only non-overlapping region access.

Client-side caching policy is a well-known technique to reduce the communication cost between clients and servers. However, in order to avoid the cache coherence problem, many file systems choose not perform this policy or lack of efficient solutions to it. We have designed a Persistent File Domain (PFD) approach, at the MPI-IO level, to solve the cache coherence problem while maintaining the caching policy performed on the clients. The idea of PFD is to partition a file into exclusive domains and assign each domain to a process. Once a process is assigned a file domain, it is responsible for delivering the data to the requesting processes for any successive I/O requests to this domain until the file is closed. Since a file domain is read/written by one process only, client-side cache coherence problem is solved. We compared the performance of using different striping factors for the domain assignment as well as with the intuitive approach that explicitly invalidating/flushing the cache at every read/write call. By using a sliding window access pattern, the PFD approach shows a significant performance improvement over the invalidating-flushing approach. This implementation is also submitted to MPICH development team for potential software incorporation into the MPICH distribution.

Benefits to Sandia

It should be noted that this research would directly benefit Cplant clusters' applications. Currently there is no mechanism that controls application nodes from overwriting results from nodes within applications. Also, it is possible to retrieve obsolete data on one node due to the caching issues mentioned above. This research will provide software that will provide controls on output and eliminate retrieving obsolete data.

It is expected that this research will result in the publication and presentation of papers to juried symposia. Scalable Implementations of MPI Atomicity for Concurrent Overlapping I/O, which resulted from Year 1 efforts, was accepted at ICPP 2003. It should be noted that only 37% of the submitted papers were accepted.

FY04 Objectives:

Objective 1. Optimizations for Persistent File Domain (PFD)

Investigate enhancements to Persistent File Domains (PFD). `MPI_File_set_view()` contains useful information that potentially can be used to further optimize the I/O performance. Since `MPI_File_set_view()` is collective, the file visible domain to one process can also be known by others in which the opportunities of I/O optimizations are expected. Contractor will investigate the use of this information together with the data access extent to determine an optimal PFD in each. Contractor will investigate dynamical re-assignment of PFD to reflect the change of the access patterns issued from the current I/O calls. Contractor will investigate I/O performance by means of MPI-IO file access.

Objective 2: Extend PFD Techniques for MPI Atomicity

Contractor will investigate incorporating the implementation for MPI atomicity into the PFD framework. Many file systems perform client-side caching together with read-ahead and write-behind strategy in order to speed up the sequential access to the file data. The size of cache buffer is usually in the unit of file blocks. A concurrent overlapping I/O request can easily result in the same file blocks cached in multiple clients where the cache coherence problem emerges. A traditional solution to this is through using the file locking mechanism to bypass the write-behind, so the file modification is visible to all cached clients. However, using file locking can seriously degrade the I/O parallelism as demonstrated in our previous work. We will extend the PFD work to cover this problem. Basically, our idea is to have an I/O request performed through the clients that cached the requesting data. Since file locking is not required in this approach, the degree of I/O parallelism can be maintained.

Objective 3: Design Cache Coherence Solution for MPI Non-collective I/O

Non-collective I/O poses a tremendous challenge to optimize I/O because different processes can perform I/O at any time and do not synchronize their requests with each other. Contractor will investigate extending the PFD approach to MPI non-collective I/O calls. Contractor will investigate PFD assignment at file open and set view since these two MPI calls are synchronous. For the implementation of non-collective I/O requests, contractor will investigate two approaches: using MPI one-side communication and using a multi-thread implementation. Contractor will also evaluate the impact of using different file block sizes to the concurrent overlapping I/O performance.

FY04 Tasks:

First quarter:

1. Develop a bookkeeping approach for tracing the change on the MPI fileview and data request size (data type for I/O buffers.)
2. Implement the PFD re-assignment.
3. Implement the trigger condition for PFD re-assignment.
4. Collect potential file hints that can be used to fine-tune the persistent file domain partitioning.
5. Determine which ROMIO codes should incorporate this optimization.

6. Evaluate I/O benchmarks to examine the effect of PFD implementation.

Second quarter:

7. Incorporate the MPI atomicity implementation to the PFD framework.
8. Study MPI one-side communication.
9. Design techniques that use the PFD concept with MPI one-side communication.
10. Identify the ROMIO code fragments for inserting our implementation.

Third quarter:

11. Implement the PFD for MPI non-collective.
12. Study the data access patterns of a few parallel scientific applications that can potentially benefit.
13. Study potential file hints, either provided from users or generated from the data types used in the program, for determining proper file domain partitioning method.

Fourth quarter:

14. Examine the connection of modified interfaces between ROMIO and MPI-IO to ensure all MPI-IO applications perform without changing their MPI-IO calls.
15. Benchmark for regular and common access patterns for PFD on non-collective I/O operations.

FYO4 Deliverables:

Quarterly Status Report and a Final Report

Title: Surrogate-Based Optimization

PI: J.E. Dennis, Jr., Rice University

Dates: July 1, 2003 – June 30, 2004

CSRI POC: Paul Boggs, (925) 294-4630

Project Summary:

The purpose of this proposal is to fund the PI's interaction with Sandia National Laboratories at NM and CA. These interactions should be of two sorts. First, algorithmic advances and interesting practical experience of the PI and his collaborators in universities and industry would be transferred to the labs, and conversely, lab problems and experience would inform the research of the PI and his collaborators. Bidirectional technology transfer is our goal and firm belief. We seek to be both brokers and developers; to provide support and receive feedback. The point of the visits for which support is requested is to increase the total pool of knowledge about engineering design problems of the particularly nasty sort discussed below.

The class of optimization problems that we target is largely from engineering design and widely regarded by practicing designers as intractable. We have focused for several years not on solving problems better, but on solving problems that can not be solved at all well by existing methods. We have resisted the temptation succumbed to by some university engineering groups of designing elaborate (soft) design support systems based on naive expectations of the spontaneous generation of supporting algorithms. Instead, we have focused on providing the rigorous mathematical infrastructure to underpin design support systems such as Boeing's Design Explorer and Sandia's DAKOTA, though to date, we have had measurable impact only on Design Explorer, where our influence has been considerable. Dr. Greg Shubin, Head of Mathematics and Engineering Analysis, or Dr Evin Cramer, Technical Fellow of Boeing Phantom Works can verify our contributions. <shubin or cramer>@redwood.rt.cs.boeing.com.

Another tenet of our research is that engineers generally understand their problems better than we can, and so while we do provide default choices, all our work has been directed by the rule that engineering intuition should be able to be seamlessly incorporated into our algorithmic framework. We take over only when the user's approach has reached the limit of its resolution, and we proceed to "clean up" the final design or to get the designer out of a rut fallen into by conventional approaches.

Our algorithms are carefully structured so that if a user has a favorite method for solving the surrogate problem, then it can be provided to our FOCUS software as a SEARCH procedure in a direct search method. Thus, we provide direct search methods to act as meta-algorithms supporting user favored heuristics. So far, we have the algorithms and software in place to deal with general nonlinearly constrained optimization for problems of the type we see often in engineering design:

f(x), C(x) are expensive and have few correct digits. This happens because there is an underlying expensive state equations that needs to be solved for a given x to generate the state variables that are used to evaluate the optimization problem functionals. Evaluation may fail (f(x)=infinity) expensively and unexpectedly for feasible x and f and C may be discontinuous even when they are defined. This happens because the state equation solver mentioned above is often a kludgey coupling of table lookups and state equation solvers from different physical disciplines. For example, one might use successive replacements to try to couple a structures solver with a dynamics solver. This procedure may work for some x, but it may not for one nearby. In a Boeing helicopter rotor design problem, the function failed to return a value about 67% of the time. Someone unfamiliar with commercial reality might suggest that the solvers should be tightly coupled to smooth out this behavior. Indeed, a part of the economic justification for making such an effort can derive from a proof of concept we might provide by the techniques suggested here. Before bandoning legacy solvers to reimplement a solver more amenable to SAND type approaches, try this approach to estimate the economic gains. Evaluation will usually fail unless some selected simple constraints hold. This happens when there are simple bounds, like nonnegativity, on some of physical parameters. It means

that we must be able to be always feasible with respect to some constraints, though for efficiency, we would like to allow infeasibilities during the course of the interaction in any constraints for which that is reasonable.

In addition, since we are usually dealing with interpolatory surrogates like polynomials, (kriging) splines, or neural nets, there is a fairly low limit on the number of decision variables we can treat. However, this is a problem with constructing interpolants more than with the underlying approach. Thus, if the surrogates come from a less detailed description of the underlying physics, then we can treat more decision variables. We are aiming for an ExxonMobil problem with a couple hundred each discrete and continuous variables, and for which the surrogate is based on a simplified model of flow-in-porous media. Still, the largest problem we actually have solved was 256 continuous decision variables.

To meet these challenges of our problem class, we have been able, for the very nice Lewis and Torczon barrier algorithm (f(x) is infinite if x is not feasible), to use a crucially different proof to strengthen their convergence results for nonlinear optimization under simple linear constraints by dropping their assumption of continuous differentiability on an open set containing the feasible region. Indeed, if the initial iterate has finite problem function values, then we show the existence of a limit point even when the functions are discontinuous and extended real valued. If the problem is locally smooth at such a point, then we show appropriate optimality conditions from the Bourbaki/Clarke nonsmooth analysis. In addition, the proofs based on our weaker hypotheses are much shorter and simpler.

Our general constrained algorithm FPS adapts Fletcher's new penalty function-free filter step acceptance idea to direct search methods. Thanks to our improved convergence analysis mentioned above, we can allow discontinuities and extended values in the function to which the algorithm is applied, Thus, we can apply our NLP filter method directly to the Lewis and Torczon barrier function and thus enforce every iterate feasibility for simple linear constraints with no need for extra complication in the theory. This FPS algorithm is being used at Boeing in the current release of the Boeing Design Explorer package. It had a great success in wing planform design.

The focus of our efforts supported by research funds will be to:

- **Implement our mixed discrete/continuous variable algorithm MVP in FOCUS during the next 3 years.** This is the longest-term goal of the proposal. The difficulty lies in the fact that our main focus is on categorical discrete variables and nonlinear nonconvex problems. These are very common in engineering design, and they are usually handled by heuristic parameter studies. For our purposes, a categorical variable is a variable, which is an input to the simulation driving the optimization, but it has the property that if its input value is not from a prescribed finite set, then the simulation will not run and the function or the constraints cannot be evaluated. This property precludes the use of continuous relaxations for discrete variables, and hence branch and bound. Our MATLAB MVP has been quite successful on some artificial test problems as well as on a problem from cryogenic engineering design from a mechanical engineer at the Automotive Research Center at Ann Arbor. In that problem, MVP increased or decreased the number of heat intercepts and changed the neighboring insulation material of as the iteration proceeded. This means that number of heat intercepts, which determines the number of optimization variables was itself an optimization variable. We were able to obtain a 60% reduction in the require power by our approach over the best published result that chose the categorical variables by a parametric study. We regard this as highly promising behavior. We continue work on the algorithm. The software difficulty is in designing a user interface to capture the user's domain specific knowledge concerning the relationships between variables like different insulation materials.

- **Extend our MVP work to generally constrained mixed variable problems**. We have long advocated using the Ferris-Mangasarian variable distribution techniques to extend our algorithms to higher dimensions. Those techniques can be thought of as an adaptive approach to the linking variables long used by design engineers and explained in the book by Vanderplaats.

- **Continue development of multiobjective filter based tools to support engineering decisions on trading off various competing objectives**. This is the holy grail. Our preliminary MATLAB experiments indicate that the surrogate/filter approach may extend current capabilities, but there is much to do here. We would like to provide a surrogate based representation of the trade-off surfaces, which we would refine as the user homes in on the interesting region.

The visits supported by this funding would aim to:

- **Work with Bill Hart on incorporation of evolutionary approaches to SEARCH for all our algorithms**. It is important to provide effective default SEARCH procedures for casual and evaluative use or for naive users. Bill Hart's work seems very well suited in robustness and general applicability to this application. The way our framework is designed, we give the user the opportunity to embed their own optimization procedures to be applied to the surrogate to identify promising candidates for improved designs. This is an important feature of our approach. Many designers have ad hoc approaches.

- **Work with Mike Eldred on algorithmic enhancements to DAKOTA**.

- **Work with Juan Meza, Paul Boggs, Patty Hough, and Tammy Kolda on enhancements to the PDS/trust-region algorithm**. Specifically, we advocate the use of the local quasi-Newton quadratic model as a surrogate, and we suggest the restriction of the SEARCH based on this surrogate to a lower dimensional subspace as in the work of Byrd, Schnabel and Schultz or in the work of Boggs, Kearsley, and Tolle.

Title: Global-Basis method for fluid problems

PI: Professor Jacob Fish

Investigator: Haim Waisman, PhD student

Dates: May 8, 2003 – September 30, 2004

CSRI POC: John Aidun, (505) 844-1209

Project Summary:

Research efforts will focus on (i) implementation of the Global-Basis method in SALSA and ML-pack and (ii) validation of the Global-Basis method on fluid problems to be provided by Sandia. The graduate student, Haim Waisman (US Permanent Resident), will be closely working with Ray Tuminaro at Livermore on ML pack issues and John Shadid on issues related to SALSA, fluid flow problems and code validation.

Haim will be faced with the following three tasks:

1. Implementation of a complex prolongation operator
2. Construction of hybrid prolongation operator consisting of combination of local and global basis vectors
3. Implementation of the Global-Basis method as a filter to the existing multilevel and single level methods within SALSA and ML-pack

Task 1: The smoothing iteration matrix is nonsymmetric and for indefinite system the spectral radius is greater than one. Therefore, the optimal prolongation operator spanning the space orthogonal to the smother may be complex. Currently, ML-pack only works with real numbers. Thus one of Haim's talks would be to work with Ray Tuminaro on generalizing the framework of ML-pack to allow for complex algebra.

Task 2: One of the multilevel versions of the proposed Global-Basis methods consists of expanding the sparse prolongation matrix based on the local basis (for example obtained from the Smoothed Aggregation method) with global basis vectors obtained from the Arnoldi method (AR-pack). This will require development of coarse level matrices from a mixture of sparse (based on local basis) and dense (based on global basis) prolongation and restriction operators.

Task 3: This task calls for the implementation of a filter within or on top of the ML-pack. Most of the local basis multilevel methods will fail for highly indefinite systems. In this implementation Global-Basis method will detect the modes which cause divergence of the iterative method of choice and will construct an additional level that will filter out the "bad" modes.

This is obviously a very ambitious program and we do not expect that within the three months of the summer program that Haim will be able to successfully complete all the goals stated in the three tasks. We hope however, that during his stay he will be able to make significant progress on the three fronts by working together with John and Ray, so that when he returns to RPI later in the Fall semester in 2003 he would be well positioned to successfully complete all the tasks.

Title: Large-Scale PDE-Constrained Optimization

PI: Omar Ghattas, Carnegie Mellon University
Lorenz Biegler, Carnegie Mellon University

Dates: October 1, 2003 – July 31, 2004

CSRI POC: Bart van Bloemen Waanders, (505) 284-6746

Project Summary:

1 Introduction

This document proposes research for FY2003–FY2004 within the PDE-Constrained Optimization Project under the auspices of Sandia National Laboratories' Computer Science Research Institute. This project is collaboration between faculty, postdocs, and students at Carnegie Mellon, Courant, and Rice Universities, and Sandia Albuquerque and Livermore researchers. The project's principal aims are to develop, implement, and demonstrate algorithms and software tools for optimization of systems governed by partial differential equations (PDEs). PDE-constrained optimization is a critical enabling technology as the engineering community moves beyond simulation to simulation-based design, control, and parameter estimation. While the field of computational nonlinear optimization has made steady progress over the past 30 years, the class of PDE-constrained optimization problems we target presents unique and pervasive challenges.

Particularly when the PDE simulations are large and complex—as embodied by Sandia's suite of large-scale production engineering simulation codes—and the optimization variables are finely parameterized, entirely new classes of scalable, efficient, and robust optimization algorithms are required. This imperative is made all the more critical by the maturing state of PDE simulation technology. For a number of problem classes, it is only now—that the mathematical models are sufficiently physically descriptive, the numerical discretizations are sufficiently robust, and the "forward" PDE solvers are sufficiently scalable to high-resolution problems—that PDE-optimization becomes not only warranted but necessary for adding the most value to simulation.

2 Research Tasks

This section describes research tasks we feel are essential for advancing the technology of PDE optimization to the point where it can be readily applied to large, complex, parallel applications typical of Sandia's suite of simulation codes. The primary mechanism for conducting this research will be through short and long term visits by university faculty, postdocs, and students to Sandia at both Albuquerque and Livermore locations.

At the same time, this research program will leverage ongoing algorithmic research at Carnegie Mellon, Courant, and Rice that is funded by other sources. The visits will help motivate and direct this work to the complexities presented by Sandia applications.

Task 1: Investigate domain decomposition approaches for time-dependent and stationary optimization problems with relevance to Sandia applications

The solution of quadratic programming sub problems is the most computationally time-consuming component of a full space SQP method. When applied to PDE constrained optimization, Krylov subspace methods combined with domain decomposition (DD) based preconditioners have proven to be successful for these tasks. One such approach we have developed, the Lagrange-Newton-Krylov-Schur (LNKS) method, as 1 implemented in the Veltisto package, preconditions by decomposing the full space of unknowns into state, adjoint, and decision subspaces, with approximate solves within each subspace in turn effected by domain decomposition preconditioners. The approach can be very effective for steady PDE optimization; for example, solution of 3D Navier Stokes optimal flow control problems with O(106) states and O(104) controls has been achieved in as little as five times the cost of the flow solution, and with high parallel efficiency. There are several remaining challenges to ensure a scalable general-purpose method for PDE optimization. First, we need better-reduced Hessian preconditioners, which at the moment are on

based on limited memory quasi-Newton ideas. We will be pursuing preconditioners based on the character of the underlying infinite dimensional operator, for general classes of problems. Second, scalable preconditioners are required for incorporating inequalities on state and decision variables. We have recently proposed such a preconditioner that for certain problems seems insensitive to barrier terms introduced by interior-point methods. We will extend and explore this DD preconditioner for a broader class of applications arising at Sandia. This complements the recent work of the project on interior-point SQP. In particular, the resulting preconditioners can be directly applied to solving tangential subproblems in MOOCHO. Third, time-dependent PDE optimization remains a formidable task, which often requires different solution techniques, than those applicable for steady state problems. We plan to continue our work that addresses these issues, both on time-domain decomposition methods, as well as on improved preconditioners for time-dependent reduced Hessians. The Sundance–MOOCHO interface will serve as a prototyping tool to explore different time-domain decomposition strategies before applying the most promising to Sandia simulation tools.

Task 2: Investigate discretization accuracy for optimization for select Sandia applications, using Sandia simulation codes and frameworks

In PDE-constrained optimization, it is often assumed that accurate PDE solvers combined with robust optimization tools are sufficient to compute accurate optimal solutions. This is often true when applied to simple test problems, but may not hold when more sophisticated discretizations are applied to complex problems. In this case, a straightforward interface of PDE solver and optimizer may compute an optimal control/design/parameter at a computational cost that is much higher than required for the quality of the computed solution or, worse, may compute a control/design/parameter that has little to do with the optimal control/design/parameter. In such cases, discretizations can sometimes be modified to remedy this inferior behavior. We have analyzed this in the context of some model problems discretized using stabilized finite elements. We will explore this issue on selected Sandia applications, such as source detection. We plan to use the Sundance–MOOCHO interface as a prototyping tool.

Task 3: Develop Eulerian methods for shape optimization

The development of efficient general-purpose algorithms for shape optimization will have a significant impact on simulation-based optimal design. However, shape optimization presents several additional difficulties beyond those encountered in non-shape PDE-constrained optimization, including the computation of shape derivatives and representation and management of large shape motion and the resulting mesh movement (which has yet to be solved cleanly in a parallel environment). As an alternative to conventional moving-mesh Lagrangian methods, we will investigate level-set like techniques for representing shape in the context of PDE-based shape optimization. Level set methods overcome the difficulties of regenerating meshes and permit topological changes that classical methods are incapable of allowing. However, most level set methods are based on controlled evolution of a pseudo-time Hamilton-Jacobi system, which 2 amounts to steepest descent solution of the reduced space optimality conditions. Instead, we are pursuing a full-space, Newton-based approach that builds on our work in fast algorithms for PDE optimization to directly solve for the optimal shape. This promises to be more robust and up to several orders of magnitude faster. Since we are dispensing with controlled evolution (which has regularizing properties), we must find alternate regularizations to render the shape problem well posed. The shape optimization work is currently being prototyped in Sundance, which gives access to MOOCHO solvers. Driving Sandia applications include aerodynamics, magneto hydrodynamics, and structural dynamics applications.

Task 4: Study the influence of inexact problem information on PDE optimization methods

PDE simulation tools used at Sandia and elsewhere apply iterative solvers, mesh adaptation, etc., to efficiently compute the PDE solution for a given set of parameters. As a consequence, if such PDE solvers are interfaced with a PDE optimization tool such as MOOCHO, the latter is not supplied with exact function values or derivative information. In some cases the error in function and derivative information can be controlled, e.g., through the setting of stopping tolerances in iterative PDE solvers. In other cases at best only asymptotic information for the error is available. We have developed a theory that allows us to integrate PDE simulations that have controllable errors with SAND optimization tools. Our approach tightens the error tolerances as needed, based on the progress of the optimization, allowing inexpensive solves whenever feasible. We will implement and study our approach in the context of the Sandia PDE

optimization environment. The effects of inaccuracies for which only asymptotic error bounds are available on the performance of optimization algorithms and on the quality of the computed solution are much less understood. We plan to explore these effects on Sandia applications using Sundance–MOOCHO, MPSalsa–MOOCHO, and other existing simulation–optimization interfaces.

Task 5: Improve barrier/filter strategy for rSQP++/MOOCHO
The superior convergence properties of the interior point code IPOPT and the initial benchmark results of the barrier and filter implementations in rSQP++ (recently renamed MOOCHO) have led to a number of proposed refinements for this strategy. Working with Andreas Waechter (IBM), a new restoration strategy has been proposed for the filter line search and we will implement multi-algorithm versions of this approach into MOOCHO over the next few months. In addition, we will investigate full space SQP algorithms with barrier and filter features to complement the reduced space features that we have already implemented. The full space option allows us to assess domain independent comparisons more directly and also leverages the work that has been done on LNKS as well as implementations and applications in Sundance. Finally, we intend to explore novel preconditioners for solving tangential subproblems in MOOCHO that can also exploit the structure of barrier terms in this subproblem, as mentioned above.

Task 6: Address optimization under uncertainty
Uncertainty quantification is a strategic element of CSRI. Through developments in MOOCHO we hope to complement these efforts by providing capabilities for robust (or multiscenario) optimization strategies. These approach lead to optimal designs and decision-making that is insensitive to changes in uncertainties in the problem definition (including model parameters, external data and inputs, or performance requirements).

Optimization formulations for multiscenario problems are currently much more expensive to solve than design optimization problems. However, in the context of SAND optimization, very efficient decomposition 3 strategies can be applied that take full advantage of parallelism as well as the features of the barrier/filter approach that we will extend in MOOCHO. With this capability in MOOCHO, we will be able to develop optimal designs quickly that are tolerant to a wide variety of uncertainty descriptions for challenging large-scale PDE-based models.

Task 7: Improve SAND optimization with existing engineering packages
Over the past three years at CSRI we have developed a hierarchy of optimization implementations to PDE based modeling tools and solvers. This hierarchy allows us to gauge how the structure of existing and developing tools can be exploited for SAND optimization. For example, the rSQP++ link to MPSalsa has led to efficient SAND optimization applications for problems with few decision variables. On the other hand, through new developments such as Sundance, much larger and more challenging applications can be considered. With the addition of barrier and filter line search strategies in MOOCHO, these implementation levels can be refined further and far less information may be required from the solver (e.g., multipliers are no longer required) than with previous methods. Therefore, we intend to extend SAND optimization to additional engineering modeling tools at Sandia.

Task 8: Target Sandia applications
The work from these tasks will be applied to a number of important Sandia applications. For these, we would like to be involved in the problem formulation and solution stages. Working with the Optimization and Uncertainty Quantification team, we plan to collaborate on (and are already becoming involved in) applications related to homeland security, including source detection in water-borne and airborne contaminant transport, and the optimization of reactive and fluid flow systems. These applications will validate the algorithmic improvements described in Tasks 1–7 and lead to extensions that apply to more challenging problem characteristics.

Title: Frontiers of modeling computational and analysis

PI: Harvey Greenberg, University of Colorado, Denver

Dates: October 1, 2003 – December 31, 2004

CSRI POC: Cynthia Phillips, (505) 845-7296
William Hart, (505) 844-2217

Project Summary:

Harvey Greenberg will work with Cynthia Phillips and William Hart to refine research ideas that will be prominent in various FY04 funding proposals. In particular, he will educate and/or brainstorm on one or more of the following topics: linear-programming/integer-programming validation/certification, computation of multiple "sufficiently structurally different" solutions to (discrete) optimization problems, multiobjective branch and bound, nonlinear branch and bound, handling uncertainty in optimization, Lagrangian methods for derivative-free optimization, sensitivity analysis, post-solution analysis, and general techniques for finding robust solutions to discrete optimization problems.

Title: Reduced-order modeling with application to chemical/biological terrorist events

PI: Max D. Gunzburger, Iowa State University

Investigator: John Burkardt, Iowa State University
Janet Peterson, Iowa State University

Dates: December 1, 2003 – September 30, 2004

CSRI POC: John Shadid, (505) 845-7876

Project Summary:

The long-range goal of the project is to develop an efficient methodology for negating or at least confining the effects of the deployment of chemical or biological agents in public environments such as airport terminals. The mechanism that will be used to meet the goal is the feedback control of the airflow in the building. Sensors that detect the deployment of an agent and heating/cooling system actuators that determine the airflow will be used as inputs and outputs in the feedback process. The connection between the inputs and outputs is partly determined through the determination of the airflow in the building. Thus, central to the effective use of feedback strategies is the realtime determination of the flow field in the building. This central step cannot be effected through traditional, large-scale simulations using, e.g., finite element or finite volume discretizations. Instead, we proposed to use reduced-order models for the flow field. These models require extensive off-line computations but typically involve very few degrees of freedom so that flow solutions can be obtained in real time.

During the period 12/1/03 to 9/30/04 we will undertake the development of a reduced-order modeling simulation capability for a problem that, although not totally realistic, contains many of the features of the problem of actual interest. The goal of the work carried out over this period is to demonstrate that the reduced-order modeling approach is viable for the purposed outlined in the previous paragraph. The specific project tasks for this time period are as follows.

1. Use our existing laminar, finite element Navier-Stokes simulations codes to generate snapshots of solutions. The problem specification, e.g., media properties, geometry including actuator distributions, etc., and constraints on actuator performance will be supplied to us by Sandia personnel.
2. Develop systematic strategies, using design-of-experiment methodologies, for the determination of snapshots for use in reduced-order modeling.
3. Use the snapshots as inputs to our existing codes to determine reduced bases; two types of reduced basis will be explored: POD (proper orthogonal decomposition) and CVG (centroidal Voronoi tessellation).
4. Use our existing codes for reduced-basis flow simulations to test the accuracy of the POD and CVT reduced bases; comparisons with full finite element approximations will be carried out for a variety of inputs to the simulations.
5. Consult on the development of new versions of our reduced basis (CVT and POD) determination codes that interface with Sandia computing environments; included in this effort is possible algorithmic modifications to aid parallelization of these codes.

The following personnel will be involved in the project: John Burkardt, Max Gunzburger, and Janet Peterson. Max Gunzburger will be responsible for the overall direction of the project and will participate in all aspects of the project; John Burkardt will be responsible for the determination of reduced bases and parallelization efforts; Janet Peterson will be responsible for the generation of snapshots and the reduced-order flow simulations. All three will be involved in the design-of-experiments aspects of snapshot generation. One trip to Sandia by John Burkardt to interface with Sandia personnel on parallelization aspects of the project is expected.

Title: Multiscale Methods in Science and Engineering

PI: Dr. Thomas J. R. Hughes
The University of Texas at Austin

Dates: January 1, 2004 - September 30, 2004

CSRI POC: John Shadid, (505) 845-7876

Project Summary:

Introduction

The numerical solution of partial differential equation systems (PDEs) arising in engineering and the applied sciences involves implicitly the elimination of spatial and/or temporal scales. The appropriate solution manifolds of PDEs are infinite-dimensional whereas numerical methods, such as finite elements, wavelets, finite volumes, finite differences, and spectral methods necessarily employ finite-dimensional approximations. Typically, the eliminated scales are 'small" and the retained ones are large." These scales essentially correspond to unresolved sub-grid scale physics that is often necessary for proper approximation of the large-scale behavior of the physical system. This can be most easily understood in a spectral context in which low wave number and /or frequency Fourier modes are retained and higher ones neglected. In many applications of physical interest, standard numerical methods, such as Galerkin approximations or central difference methods, fail under these circumstances because important interactions between small and large scales are precluded. Examples are shock wave propagation and turbulence in which various somewhat ad hoc procedures have been developed. These methods have been used over the years to account for missing or unresolved effects, namely, proper entropy production in the former case and reestablishment of the energy cascade in the latter. These add-hoc modifications while attempting to provide reasonable physical behavior of the large-scales modify the basic underlying equations and can often produce a mathematically inconsistent formulation of the problem. Many other examples can be mentioned.

The variational multiscale method was developed to provide a framework for the development of numerical methods in which the effects of small scales are identified and accounted for ab initio. The first study focused on the finite element method and showed how so-called stabilized methods could be derived from fundamental principles. Stabilized methods had been shown to be effective in various circumstances previously, but were derived by ad hoc means. The variational multiscale method demonstrated that there was a solid foundation to these methods and provided a way for systematically developing them for more complex applications. In fact, it may be said that most all stabilized methods to date do not appropriately take account of nonlinear effects. Consequently, there is an opportunity to systematically explore the variational multiscale concept in a broad spectrum of important nonlinear applications. This is the intent of the proposed research. Potential benefits include upgrading the performance of existing production codes based on stabilized methods, correcting deficiencies noted in current codes, providing a rationale for and refining ad hoc techniques currently used in practice, and developing new systematic and fundamentally sound methods for applications which have not been successfully dealt with heretofore. The work to be performed under the direction of Dr. Thomas Hughes at the University of Texas at Austin will be done in collaboration with Sandia National Laboratories personnel, namely Drs. John Shadid, Pavel Bochev, Mark Christon, and David Gartling, among others. In addition, Dr. Hughes will spend time in residence at Sandia National Laboratories and will teach a short course there on the multiscale methods. The collaborative research, which is viewed as broad-based and long-term, will address the following areas.

Proposed topics

1) Shock Hydrodynamics (Sandia technical lead: Dr Mark Christon)

We will investigate: 1) the physical and numerical aspects of the von Neumann - Richtmeyer viscosity in a multiscale Lagrangian framework, and 2) develop suitable multi-dimensional models for the closure terms that derive from the multiscale variational formulation, but that are not currently included in the von Neumann viscosity. Finally, extensions to an Eulerian formulation will be developed that are suitable for treating multi-material problems. The proposed work will be demonstrated initially on suitable Lagrangian strong-shock problems and will be documented in an archival publication.

2) Compressible and Incompressible Navier-Stokes Equations and Turbulence (Sandia technical leads: Drs. John Shadid, Pavel Bochev and David Gartling)

We intend to pursue the development, implementation and analysis of a sequence of multiscale methods for transport/reaction systems. The eventual target application is the Navier-Stokes equation with thermal energy and mass transfer with chemical reactions. The major component systems will be: 1) Incompressible Navier-Stokes, 2) Navier-Stokes, thermal energy with Boussinesq interaction model, 3) Navier-Stokes, thermal energy and mass transfer with chemical reactions, 4) Compressible Navier-Stokes with a low Mach number assumption, 5) Navier-Stokes compressible flow. This effort will attempt to derive the appropriate multiscale interaction models for these systems and provide consistent turbulence models to include relevant physical mechanisms.

3) Viscoelastic Fluid Systems (Sandia technical lead: Dr. David Gartling)

We have a further interest in pursuing multiscale models for viscoelastic fluid systems. This effort will consider velocity, pressure and stress formulations. Additional efforts will attempt to couple thermal energy transport. Formulations for specific constitutive models will be pursued.

4) Large Deformation Solid Dynamics (Sandia technical lead: Dr. Mark Christon)

Multiscale and stabilized method analysis will be applied to large deformation solid mechanics problems. These methods will allow a broad choice of basis functions in contrast to classical mixed finite element methods. It will also provide an initial basis for a consistent formulation of unresolved sub-grid scale physics in a few selected applications. Possible applications include microstructure issues with PZT, and macro-scale deformation of bodies with unresolved cellular microstructure.

5) Additional Topics (Sandia technical lead: Dr. Pavel Bochev)

Possible extensions of the multiscale variational formulation to control-volume schemes, discontinuous Galerkin methods, semi-conductor device modeling with drift diffusion and hydrodynamic models, and plasma simulations will be addressed.

Tasks for FY04

1) Continue multiscale work on incompressible Navier-Stokes equations.
2) Continue multiscale work on compressible Euler equations with particular reference to artificial viscosity.
3) Continue development of stabilized mixed formulations for the drift diffusion model of semiconductor devices.

The research tasks and deliverables will be the responsibility of Dr. Hughes who will be assisted by one full-time graduate student.

Title: CSRI Executive Board Member

PI: Deepak Kapur, University of New Mexico

Dates: October 1, 2003 – September 30, 2004

CSRI POC: David Womble, (505) 845-7471

Project Summary:

The CSRI Executive Board will consist of 6-8 people representing both technical contributors and programmatic stakeholders of the Institute. This will be on a part-time basis. The responsibilities of the Executive Board member activity for Dr. Kapur are as follows:

1. Executive Board Participation

Attend regular Executive Board Meetings

Attend any special Board meetings required to meet ad hoc activities

Provide programmatic guidance and advice in regards to selection of CSRI applicants for the CSRI activities.

Actively seek staff, research programs and facilities that are highly visible and respected in computer and computational science community. Build on this reputation by actively recruiting recognized and respected university researchers to participate in the CSRI.

2. Student Research

Continue to Investigate the use of Dixon resultant based method for solving nonlinear polynomial equations.

Parallelize the code developed for solving nonlinear polynomial equations

Study how homotopy and eigen-value based methods can be adapted to exploit algebraic information available through Dixon resultant formulation.

Deliverables:

Periodic reports in the form of publications will be provided.

Annual one page report summarizing the accomplishments, benefits to Sandia National Laboratories and publications that have resulted from work performed.

Title: High End Application-Driven Architecture Research

PI: Peter M. Kogge
University of Notre Dame

Investigator: Richard Murphy and Arun Rodrigues
University of Notre Dame

Dates: May 2004 – September 2005

CSRI POC: Keith Underwood, (505) 284-9283

Project Summary:

In recent years, the so-called "memory wall" (the ratio of latency to main memory to the cycle time of a modern high performance CPU) has had a dramatic effect on the design of computers at all levels. At the desktop level, up to three levels of caches and faster memory busses have been unable to keep up with the growing disparity. At the supercomputer level, attempts to not only allow access to very remote memories, and still support some sort of memory coherence has overwhelmed interconnection bandwidth. The situation is so bad that efficiencies of only a few percent are "typical." New programming models and languages, such as MPI, co-array Fortran, etc, have by themselves added only incremental improvement.
One alternative, termed "Processing-In-Memory," has the potential to significantly affect the wall directly. With this technology, significant processing logic can be placed literally next to main memory arrays (on the memory chips themselves). Tremendous reductions in latencies are coupled with tremendous bandwidth increases to these local memories.

If used in conventional computing models, these features should allow some improvement in the situation. However, if used with new models of execution, these PIM technologies hold the potential of near revolutionary improvements in high end computing systems, especially as we move into massive parallelism. At the very simplest, the ability to expand memory access requests to include atomic "operate at the memory" radically simplifies access and updates to shared data structures. At an intermediate level, the ability to initiate a method invocation directly in the memory holding an object, and have it executed there (where latencies are short, and access to all components of the object can be done without network traffic), has the potential to eliminate many latency causing events totally, and reduce others from expensive two-way latencies to simpler one-way trips. At an even more significant level, the ability to devise architectures that support extremely light-weight threads, that can be executing remotely at a memory node and then literally "pick up and leave" when the next object referenced is not local, have the potential to radically change the way we think about memory versus processing, particularly when dealing with exactly those sparse data structures that so bedevil current supercomputers.

Over the last decade, Notre Dame has become a leader in such PIM architectures, especially when targeted to the high end of computation, as in the DIVA, HTMT, and HPCS Cascade projects. In 2003 Notre Dame, under a grant from Sandia, and with the placement of two Notre Dame graduate students for the summer at Sandia, applied several PIM-oriented simulation and analysis tools to Sandia applications, and developed some initial insight as to how Sandia-class applications might map onto PIM-based systems. Several papers based on this work were developed in collaboration with Sandia researchers, and submitted for publication.
This proposal endeavors to leverage this overall experience, especially that with Sandia, in directions of direct interest to Sandia.

Objectives and Work Descriptions
The general objectives of this project are to continue the analysis of very high end Sandia applications, but with the expanded goal of exploring and quantifying the design space for future high end PIM systems that mesh well with such applications. Specifically, there are two separable topics, discussed individually below.

Objective/Task 1: Application Mapping to a PIM-Based Memory System
To successfully deploy a large-scale PIM system, it is critical to understand the memory characteristics of large-scale Sandia applications in detail. Of particular interest are the answers to the following three questions:

Within an MPI rank, what opportunities are there to use PIMs to significantly enhance memory performance?

For Sandia applications which exhibit low temporal reuse, how do PIM-enabled heterogeneous systems (such as a possible "PIM enhanced" Red-Storm) compare to homogeneous PIM systems?
For a heterogeneous system, what opportunities are there to partition the application so that both the PIMs and the commodity processors are effectively utilized in each node?

To begin to answer these questions, detailed memory hierarchy simulations will be performed. These simulations will consist of both trace-based and execution-driven simulation. For the trace-based simulation, existing traces will be analyzed to determine the size and composition of their working set (how many opportunities for temporal and structural reuse are available, etc.). Using this analysis, a subset of memory hierarchy design point will be chosen for longer, more detailed simulation.

MicroArchitectural Enhancements
A separate question deals with how can we optimize the internal microarchitecture and ISA of a PIM system to reflect what we have learned about Sandia applications. This includes at least three specific topics: the nature of floating point operations executed "at the memory," extracting additional levels of parallelism, and optimizing MPI performance on PIM-based systems.

Floating point Computations
PIM potentially enable a variety of different computational paradigms. One of these may be to enable novel configurations of floating point processors. The PIM's wide word structure may lend itself effectively to short vector operations or to more elaborate WACI instructions (Wide ALU Control Instructions) that condense a number of FP instructions in a MIMD-like encoding which can be efficiently transferred to a FPU). In such configurations, the ratio of Integer to FP processors does not have to be one-to-one. It may be possible and efficient for several integer pipelines to ``share" a large FPU. This would allow the cost of a complex WACI, vector, or out-of-order FPU to be amortized over several processors.

We propose to explore the effectiveness of these alternative floating point architectures, and how they would apply to existing workloads while requiring little or no change by the programmer.

Extracting Additional Parallelism
Multithreaded PIMs, such as Notre Dame's recent PIM Lite chip, open up new opportunities for parallelism. However, expressing this parallelism effectively is a difficult task for the programmer and one which potentially detracts from their primary task of constructing the program. Ideally, the compiler should be able to find appropriate parallelism with at little input from the programmer as possible. Two mechanisms which potentially allows this are OpenMP and the extraction of small 'threadlets'.

'Threadlet' extraction entails extracting threads much smaller than conventional architectures can effectively utilize, often threads on the order of 5 or 10 instructions. Our preliminary work has shown that many of Sandia's scientific applications lend themselves to effective threadlet extraction.

Applying OpenMP to PIM will entail new tradeoffs, as thread overheads are different, and the partitioning of computation between PIMs and conventional processors may require new organizations of threads and new extraction procedures. Both of these techniques do not preclude the use of existing parallelism techniques - specifically MPI. We propose to explore the interaction of all of these techniques on a PIM architecture, using existing applications.

MPI
Early work showed that implementation of MPI can benefit from a number of techniques enabled by PIM such as multithreading and wide-word data transfers. We propose to continue investigation of these techniques and to explore new enhancements to MPI enabled by PIM. Three foci of investigation are the use of fine-grain synchronization to pipeline message transfer, the optimization of collective operations, and tradeoffs enabled by greater flexibility in making surface-volume tradeoffs.

Time Frames and Personnel
This project is envisioned as being staffed by two graduate students, each developed to one of the tasks, who would be in residence at Sandia.

In particular, for the first "Application Mapping to a PIM-Based Memory System" task, one graduate student, expected to be Richard Murphy, would be present at Sandia for approximately 4 months, from May 15 through Sept. 15.

For the second task, "Extracting Additional Parallelism," another graduate student, expected to be Arun Rodrigues, would spend approximately one year at Sandia, starting nominally May 15, 2004, and running through May 14, 2005.

A third student, to be identified later, may be placed at Sandia to follow up on the most promising results in the May 15-Sept 14 time frame of 2005.

Outcomes
Outcomes from this work will include Sandia Reports and technical publications authored by the students under the guidance of their professor, Dr. Kogge, and the technical staff at Sandia. In addition, simulation infrastructure developed by the students while at Sandia will be made available for continued studies. It is also assumed that during this time any results that are derived are open for publication, except of course for that material subject to government classification.

Title: Optimization Under Uncertainty

PI: John E. Renaud
Professor of Aerospace and Mechanical Engineering
University of Notre Dame

Investigator: Victor M. Perez
Harish Agarwal

Dates: August 15, 2003 – May 31, 2004

CSRI POC: Mike Eldred, (505) 844-6479

Project Summary:

Overview: This proposal involves three participants currently working at the University of Notre Dame. Professor John E. Renaud will be on a leave of absence from Notre Dame and will visit Sandia National Laboratories during the fall semester (August 22, 2003 – January 6, 2004). Victor M. Perez, who will defend his doctoral dissertation at Notre Dame this spring, and will begin working at Sandia as a post-doctoral researcher beginning June 1, 2003 and continuing through May 31, 2004. Mr. Harish Agarwal will be participating as a summer graduate student intern beginning on June 1, 2003 and working through December 31, 2003. The focus of this research participation is in the general areas of optimization algorithm development, surrogate models and uncertainty estimation.

The integration of uncertainty estimation within a framework of numerical optimization, under uncertainty offers designers new tools for validating and certifying improved designs in a simulation based design environment. Sandia is moving toward an engineering process in which decisions are increasingly based on computational simulation. In the absence of physical testing, the validation of these computational models, and the certification of designs generated by these simulation tools, remains an imposing challenge. During their stay at Sandia, participants will address the modeling of uncertainty in systems whose complexity results from the interaction of multiple disciplines. These uncertainties will be integrated in a variety of approaches for optimization under uncertainty, including the interior point trust region model management approach developed by the participants at Notre Dame (Perez, et al., 2002, Rodriguez, et al., 2001). The goal is to develop an approach for optimization under uncertainty that accounts for both epistemic uncertainties (i.e., model form uncertainty) and aleatory uncertainties (variational uncertainty in materials and manufacturing). This work builds on the strengths of each of the participants. Multilevel parallel optimization methods for simultaneous analysis of disciplines will used to drive reliability-based design optimization approaches.

Background: Dr. Renaud's experience includes five years as a manufacturing systems design engineer with the Eastman Kodak Company. He is a National Science Foundation National Young Investigator Award winner. He is currently the ex-officio chair of the AIAA Multidisciplinary Design Optimization Technical Committee. He is also a member of the executive committee of the ASME Design Automation Committee and served as the Conference Chair for the 27th ASME Design Automation Conference. He is an associate editor of the *ASME Journal of Mechanical Design* and serves on the editorial boards of *Engineering Optimization* and the *AIAA Journal of Aircraft*. His research activities include design optimization, simulation based design, uncertainty modeling, multidisciplinary design and rapid prototyping. Funding in support of his research efforts has come from the National Science Foundation, NASA, Wright Laboratories, General Electric, General Motors Corporation, Ford Motor Company, Parametric Technology Inc., Stratasys Inc., and Andersen Consulting.

Victor Perez is a Ph. D. candidate at the University of Notre Dame. He came to Notre Dame as a Fulbright fellow. His research in the areas of reduced order approximations, simulation based design, and multidisciplinary optimization has been developed under the direction of Dr. John E. Renaud. He has published eight conference papers and three journal papers in the area. His experience includes four years

as product development engineer at Robert Bosch, Mexico, and 3 years as instructor at the Iberoamericana University in Mexico City.

Harish Agarwal completed his undergraduate education in Mechanical Engineering in June 2000 from the Indian Institute of Technology (IIT), Kharagpur, India. Since then he has been pursuing graduate studies (Ph.D.) in Mechanical Engineering at the University of Notre Dame. His research interests include design optimization, simulation based design, robust design, multidisciplinary design, uncertainty modeling, reliability based design optimization and optimization under uncertainty. Currently he is working on projects involving reliability-based optimization and uncertainty modeling using evidence theory.

Potential Collaborations: The participants plan to work with the following Sandia National Laboratory scientists and engineers as part of this visit: Michael S. Eldred, Anthony A. Giunta, Scott A. Mitchell, Steven F. Wojtkiewicz, Timothy G. Trucano, Laura P. Swiler, William L. Oberkampf, Vicente J. Romero.

Dr. Michael Eldred will serve as the primary technical contact during the participant's stay. As part of his visit Dr. Renaud will present two seminars related to his research efforts in 1.) trust region model management for sequential approximate optimization and 2.) uncertainty quantification using evidence theory in simulation based design optimization. In addition Dr. Renaud will develop and offer a short course on multidisciplinary design optimization methods. Participants will have an opportunity to work with and support the development of Sandia's Dakota Framework for optimization and uncertainty analysis.

Introduction: Optimization Under Uncertainty – Reliability-Based Design Optimization
In deterministic design optimization, designs are often driven to the limit of the design constraints (active constraints at the optimum), leaving little or no latitude for uncertainty in the mathematical modeling and simulations. In addition, deterministic design optimization does not account for the variational uncertainty associated with the randomness of physical quantities that make up the system. Optimized designs determined without due consideration of variability can be unreliable leading to early life cycle failures. To account for physical uncertainties and simulation model uncertainties the use of reliability analysis must be incorporated within the design optimization process.

In the past ten years increased emphasis has been focused on the development of procedures to combine design optimization techniques with probabilistic analysis/design methods. Many new methods have been suggested by researchers for reliability-based design optimization (RBDO) such as the performance measure approach (PMA) and the reliability index approach (RIA). Variants of PMA and RIA include the advanced mean value (AMV) method, conjugate mean value (CMV) method, moving least square (MLS) method and the hybrid mean value (HMV) method (see Choi and Youn, 2001 and Choi et al., 2001). Each of these variants provides a numerical tool for probabilistic constraint evaluation. An innovative framework for reliability based multidisciplinary design optimization is developed in Sues and Cesare, 2000 and modified in Sues et. al 2001. Pettit and Grandhi, 2000 have investigated the reliability-based design optimization of aerospace structures. Qu et. al., 2000 have investigated the use of response surface approximation for reliability-based optimization of composite laminates.

Advances in Reliability Based Design Optimization
In Agarwal and Renaud, 2002, a reliability based design optimization (RBDO) framework is developed for structural design applications. The framework accounts for variational uncertainties in the structural materials used in design. Performing non-deterministic design optimization under uncertainty requires approximately n^2 additional CPU time, where n is the number of design variables, as compare to deterministic design optimization. The RBDO framework of Renaud and Agarwal makes use of response surface techniques to significantly reduce the computational cost of performing reliability analysis. The resulting designs perform robustly with respect to the variability in the material properties of the system.

Variational uncertainty, which is associated with the randomness of physical quantities, is easily modeled by statistical means using probability and cumulative density functions. *Model and simulation uncertainty are much more difficult to characterize and have to be modeled using other means such as possibility theory, fuzzy sets, evidence theory, etc Oberkampf et al., 2001.* In Agarwal, et al., 2003, evidence theory is

used to account for model and simulation uncertainty in multidisciplinary design optimization. Performance constraints are formulated using *belief and plausibility measures* developed using evidence theory. Evidence theory has received considerable attention in recent years from scientists at Sandia National Laboratories, where all designs must be certified through the exclusive use of modeling and simulation. This work builds on the earlier efforts of Gu et al., 2000 in which a robust design optimization strategy is developed. In that study a methodology for estimating worst case propagated uncertainties in coupled multi-physics systems is developed. The worst case propagated uncertainties account for both the variability in physical quantities as well as the epistemic uncertainties (i.e., bias errors) in the numerical simulations used to drive the design process.

In Gu and Renaud, 2001, 2002 an implicit approach to modeling uncertainties within a multilevel optimization framework is developed. The multilevel optimization framework makes use of decomposition and therefore does not enforce consistency of the multidisciplinary analyses during the optimization. Implicit methods are required in order to estimate uncertainties.

Evidence Theory for Estimating Simulation Uncertainties

The reliability index approach discussed earlier does not account for uncertainties in the simulation models used to drive the optimization process. In general, a distinction can be made between aleatory uncertainty (also referred to as, variability, stochastic uncertainty, irreducible uncertainty, inherent uncertainty), and epistemic uncertainty (also referred to as model form uncertainty, reducible uncertainty, subjective uncertainty, or simply *uncertainty*) (see Oberkampf et al., 1998, 1999 2001). Material and manufacturing variations (aleatory uncertainties) can be modeled using probabilistic methods. While the uncertainty in simulation models (epistemic uncertainties) must be modeled using other mathematical theories, distinct from probability theory.

Agarwal et al., 2003 focuses on accounting for uncertainties in mathematical models (i.e., simulation tools) used for non-deterministic engineering systems design and optimization. The non-deterministic nature of the mathematical model of the system exists from the fact that: a) the system responses of the model can be non-unique due of the existence of uncertainties in the input parameters of the model, or b) there are multiple alternative mathematical models for the system and the environment. The simulation tool, however is deterministic in the sense that given the same input data, the simulation tool gives unique values of response quantities.

Agarwal et al., 2003 model epistemic uncertainty using the theory of belief measures, popularly known as *evidence theory* or *dempster-shafer theory* (see Klir and Wierman, 1998, Parsons, 2001). The advantage of using evidence theory lies in the fact that it can be successfully used to quantify the degree of uncertainty when the amount of information available is sparse. Like most modern uncertainty theories, evidence theory provides two uncertain measures. They are known as belief and plausibility. In Agarwal et al., 2003 the use of these uncertain measures are used to model non-deterministic performance constraints within a design optimization framework.

As part of this activity, the evidence theory approach developed in Agarwal et al., 2003 for optimization under uncertainty will be combined with traditional reliability approaches which account for aleatory uncertainties, in optimizing multidisciplinary systems. This approach will account for both the variation in material properties and manufacturing (aleatory uncertainty) and the imprecision in the simulation tools (epistemic uncertainty) developed for multidisciplinary design.

Single Level Method Development for Optimization Under Uncertainty

Many reliability based design optimization methods are typically nested (i.e., multilevel) optimization frameworks. The significant computational expense in evaluating reliability constraints derives from the fact that the constraint *reliability analysis* methods are themselves formulated as an optimization problems (Rackwitz, 2000). To overcome this difficulty, single level approaches have been proposed in Kuschel and Rackwitz, 2000, Wang and Kodiyalam, 2002, and Chen et al., 1997. Single level reliability based optimization problems can be formulated in two different ways. In one of the approaches, the reliability constraints (lower-level optimization) are replaced by Karush-Kuhn-Tucker (KKT) optimality conditions for the first order reliability problem (Kuschel and Rackwitz, 2000). This formulation suffers from some

serious drawbacks. First, it requires Hessian information of the limit-state functions, which leads to the failure of the traditional optimization algorithms. Second, an explicit transformation from the standard normal space to the original space of random variables is necessary. Third, it is also limited to FORM and SORM approximations. The other single level approach appears to offer improved efficiencies. This formulation completely eliminates the lower level optimization of the constraints and the most probable point (MPP) of failure is instead determined implicitly as the algorithm proceed towards the optima in a single level iterative fashion Wang and Kodiyalam, 2002. *The development of computational improvements in single level reliability based design optimization will be investigated during the participant's visits.*

The participants are currently investigating the use of multilevel parallel optimization methods for the simultaneous analysis of disciplines within the Wang and Kodiyalam method. Initial results indicate significant computational savings when using the multilevel parallel optimizer as a driver. The method can be implemented in parallel and the opportunity to work with the parallel computation capabilities of Sandia will benefit this research.

Test Problems

Dr. Renaud's laboratory at the University of Notre Dame has access to a suite of smaller test problems for validating new numerical optimization methods. The opportunity to work with larger test problems available at Sandia such as the ICF capsule design problem is very appealing to the investigators. Dr. Renaud's laboratory has been developing a morphing aircraft optimization test problem involving an unmanned arial vehicle (UAV). The fully unstructured Navier –Stokes code FUN2D developed at NASA is used for the CFD analysis of the aircraft's performance.

Summary

The focus of this research participation is in the general area of optimization under uncertainty (OUU). This collaborative effort will allow the participants to investigate and develop a variety of methods including new parallel methods for simultaneous analysis within the OUU approach of Wang and Kodiyalam. The use of reduced order surrogate models within an interior point approach for optimization under uncertainty will be investigated. The use of evidence theory for estimating model form uncertainty combined with probabilistic methods to account for aleatory uncertainties within an OUU framework will also be investigated. This research will exploit the parallel computational capabilities available at Sandia. Personnel at Sandia will have an opportunity to attend seminars and a short course offered by the participants. The integration of uncertainty estimation within a framework of numerical optimization, under uncertainty offers designers new tools for validating and certifying improved designs in a simulation based design environment.

Title: Large Scale Eigenvalue Methods and Model Reduction of Second Order Systems

PI: Dan C. Sorensen, Rice University

Dates: October 1, 2003 – September 30, 2004

CSRI POC: David Womble, (505) 845-7471

Project Summary:

Large Scale Eigenvalue Problems - We shall continue to develop techniques for improving the performance of ARPACK. This software for large eigenvalue problems is in wide use at Sandia and is based upon our implicitly restarted Arnoldi method. We hope to develop pre-conditioning techniques appropriate for stability and bifurcation analysis of dynamical systems. These will be closely related to the use of iterative methods for solving the equations required to implement a Cayley transformation. However, they will construct a fixed (preconditioned) polynomial operator as an approximation to the shift-invert operator.

Model Reduction of Second Order Dynamical - Systems Direct numerical simulation of dynamical systems has been an extremely successful means for studying complex physical phenomena. However, as more detail is included, the dimensionality of such simulations may increase to unmanageable levels of storage and computational requirements. One approach to overcoming this is through model reduction. The goal is to produce a low dimensional system that has the same response characteristics as the original system with far less storage requirements and much lower evaluation time. The resulting reduced model might be used to replace the original system as a component in a larger simulation or it might be used to develop a low dimensional controller suitable for real time applications.

In the past year, we have made considerable progress on the fundamental model reduction of systems of the form $\dot{x} = Ax + Bu,\ y = Cx$ where *A, B, C* are real $n \times n,\ n \times m$ and $p \times m$ matrices, while *u, y, x* are vector valued functions of time. Large systems of this form arise in many applications, for example in circuit simulation and in the simulation of PDEs. We have developed balanced model reduction techniques for large-scale systems through low rank approximation of certain system Grammians. These techniques are matrix-free in the same sense as Krylov methods for eigenvalue computation and solution of linear systems. Balanced reduction is an excellent candidate for the development of robust and widely applicable software because of the existence of *a-priori* error bounds and the preservation of important system properties. We intend to extend these results and also develop new techniques for model reduction of second order systems $M\ddot{x} + G\dot{x} + Kx = Bu,\ y = Px + Q\dot{x}$.

Such systems are far more challenging to work with but they have many more applications. Moreover, even though a second order system can be reduced to a first order system through standard techniques, a reduced model obtained from the first order formulation is usually not valid when converted back to the second order setting. We hope to develop balanced model reduction techniques that work directly with the second order system.

Title: The Red Summit Project:
Petaflops Scale Computing through Processor in Memory Architecture

PI: Dr. Thomas Sterling, California Institute of Technology

Dates: October 1, 2003 – September 30, 2004

CSRI POC: Erik DeBenedictis, (505) 284-4017

Project Summary:

Introduction

The California Institute of Technology seeks to renew and continue its successful research collaboration with the Sandia National Laboratory in the area of advanced high end computing architecture. Caltech is currently completing a two-year research project sponsored by the CSRI to explore the opportunity of achieving performance gain for MPPs through the augmentation of such systems with advanced processor in memory or PIM components substituted for at least part of the system main memory. Significant progress towards this goal has been accomplished through the Caltech project although additional work is required to fully satisfy all of the original program objectives. As a result of this effort, significant potential has been demonstrated, not just for PIM-enhanced MPPs but also for large arrays of PIM components alone. Caltech proposes to actively collaborate with Sandia National Laboratory to aggressively pursue this important opportunity with CSRI towards the goal of accelerating the path to practical Petaflops-scale computing, for possible delivery well within this decade. This proposal constitutes a request for one-year renewal and extension of the existing project to complete its goals and to establish a three-way working relationship combining the interests and talents of CSRI, Caltech, and the University of Notre Dame towards the potential opportunity of PIM technology for real world applications. This proposal is being submitted in conjunction with a second proposal to CSRF to conduct a parallel effort in detailed system studies related to implementation, integration, and application of PIM.

Towards a PIM Petaflops Computer Architecture

PIM combines computing logic and memory stacks on the same integrated semiconductor die. Structures enabled by this merger permit low latency access to data stored in memory, simultaneous access to data contents of an entire memory row (typically 256 bytes), and the opportunity to partition the total memory capacity of a single chip in to many memory/logic nodes (potentially 64 by 2005) to greatly expose and exploit on-chip memory bandwidth and provide high degree of concurrent execution on a single die. Estimates of potential peak performance vary significantly but 64 Gflops peak performance per chip is a reasonable estimate (+/- 50%) with half a Gbyte of memory in the second half of this decade. Computation performed by such a system is very different from conventional clustered solutions. Instead of a process residing on a single node, many threads of computation will be performed concurrently, migrating through memory by means of parcels between nodes and threads on each node. The node processors themselves perform as fine grain transactional processing elements in response to incident parcels and sharing a virtual global address space with all other PIM chips and nodes. This demand driven paradigm is highly adaptive at runtime, automatically overlaps communication with computation, and exposes a fine grain application parallelism intrinsic to sparse irregular data structures. It also permits flexibility in architecture by allowing the integration of shared functional units with a PIM chip to be dynamically scheduled on a fine grain basis. It is the relationship of the new computing model enabled by this advanced PIM concept to important applications and the opportunity to exploit shared functional units that are the focus of this one-year proposal to SNL CSRI.

Proposed Project Goal and Objectives

The goal of the proposed Red Summit Project is to enable and accelerate the realization of practical effective general-purpose Petaflops-scale computation in the earliest time frame for DOE applications critical to national security and industrial commerce. Implicit in this goal is the need to achieve breakthrough innovation in scalable computer architecture and its application to real world problems. To

achieve this goal, the Red Summit Project is being proposed to make distinct and complementary advances within a broader context of research that is exploring a set of interrelated concepts. Within this research framework, the Red Summit Project will investigate two key aspects of the challenge: exploiting separate functional units and applying the architecture to key applications. Therefore, the objectives of the Red Summit project are:

1. To achieve a detailed understanding of the effect of the MIND architecture on key applications, and
2. To understand how to incorporate semantic hooks in to the evolving MIND instruction set architecture in order to exploit various "drop-in" functional units that may be shared among multiple MIND nodes on a given chip.

An important aspect of this proposal is the nurturing of close collaborations and frequent interactions with research scientists at Sandia National Laboratory. Experience with the first project shows that even in spite of best intentions, without mutual interest and involvement of both institutions, effective communications will be limited and visits fewer than desired, even as their value is less than wished. To address this challenge and build a strong collaboration with close interactions, the partnership described above will provide specific shared tasks, identified points of contact, and visits by SNL scientists to Caltech as well as visits by Caltech scientists to Sandia. In addition, Caltech will organize a small workshop on the emerging technology under separate Sandia sponsorship. Finally, as has been the case in the past, the PI and Caltech colleagues will actively contribute to Sandia hosted workshops in topics related to high end computing throughout the duration of the project award period.

Project Tasks

The tasks specified below are those to be conducted explicitly under sponsorship of Sandia National Laboratory in coordination with CSRI and do not represent the entire body of work being performed related to the goals of this project under separate contract as discussed above. The tasks are focused on achieving coordinated and cooperative research of strong interest to both institutions and engaging key researchers in a strong collaboration. In particular, it is intended to work directly with SNL computational scientists in the development of application codes that can run on the MIND architecture and to port such codes on to the MIND FPGA prototype when it becomes available. This work was begun during the first CSRI research project on one such application, LJS. It is also intended to work with SNL scientists in the extension of the MIND instruction set to provide extensible logical interfaces to shared functional units.

Year 1

1. Collaborate with SNL scientists to develop instruction set architecture extensions for support of external functional units and test on the MIND prototype.
2. Develop two application codes of significance to SNL, and port them to run on the MIND prototype.

Title: Progressing from Linearly Constrained Pattern Search to Nonlinearly Constrained Pattern Search

PI: Robert Michael Lewis and Virginia Torczon
College of William and Mary

Dates: May 15 - December 31, 2004

CSRI POC: Bill Hart (505 844-2217 and Tammy Kolda, (925) 294-4769

Project Summary:

Goals

- Distribute to Bill Hart (Sandia, Albuquerque) and Tammy Kolda (Sandia, Livermore) the C/C++ implementation of robust pattern search to handle problems with degenerate linear constraints. This is the joint work by Michael and Virginia (supported, in part, by previous DOE contracts) with Anne Shepherd, who enjoys a DOE High-Performance Computer Science Graduate Fellowship supported by the CSRI through the Krell Institute.
- Present to Bill Hart ideas for a new framework for handling search algorithms in a distributed computing environment and work on establishing protocols for general, extensible software tools. The goal would be to see if approaches, specific to pattern search, currently being developed by Anne Shepherd under our joint supervision could be generalized to cover a wider class of optimization algorithms.
- With Tammy Kolda, revise for SIAM Journal on Optimization the paper "Stationarity results for generating set search for linearly constrained optimization," written under prior CSRI contracts and released as Technical Report SAND2003-8550.
- With Tammy Kolda, use the results in TR SAND2003-8550, which cover the linearly constrained case, to derive results for general nonlinear constraints. The goal would be to develop both a general algorithmic form, and the accompanying convergence analysis, and write this up for submission to SIAM Journal on Optimization.
- With Tammy Kolda, initiate an investigation of efficient ways to extend extant pattern search software (APPSPACK, in particular) to handle general nonlinear constraints.

Context

This year we continue our investigation of pattern search algorithms for solving the nonlinear programming problem

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } x \in S \end{aligned} \tag{1}$$

where $f: \mathrm{R}^n \rightarrow \mathrm{R}$ and $A \in \mathrm{R}^m \times \mathrm{R}^n$. Recent efforts [9, 10, 13] have focused on the linearly constrained case

$$\begin{aligned} &\text{minimize } f(x) \\ &\text{subject to } Ax \leq 0 \\ &\qquad \ell \leq x \leq u, \end{aligned} \tag{2}$$

where $f: \mathrm{R}^n \rightarrow \mathrm{R}$ and $A \in \mathrm{R}^m \times \mathrm{R}^n$.

This year we will deliver a prototype C/C++ implementation for handling the special case of linear constraints. The prototype implementation does handle the case of degenerate constraints (which can occur in practice). From the start, we have known that our analysis covers the case of degeneracy [16, 9, 10], but it is well-known from linear programming that degeneracy is inherently difficult to handle in practice. Getting an implementation for pattern search that produced correct results in the presence of degeneracy, a task that has consumed most of Anne Shepherd's time between January 2003 and January 2004, proved to be more complicated than we had originally anticipated. Nevertheless, we now have a working implementation that correctly handles all the degenerate problems we have tested. We are in the process of

writing up a description of the implementation for submission to SIAM Journal on Scientific Computing [13]. In addition, Anne is in the process of revising the first implementation in light of what we now understand to be necessary to ensure that the implementation works correctly in the presence of degeneracy.

Both Bill Hart and Tammy Kolda have expressed interest in this work. Tammy has the immediate goal of overseeing the integration of the procedures for handling degenerate constraints into her latest version of APPSPACK.

The plan is for Anne Shepherd to spend the summer of 2004 at CSRI, Sandia, Albuquerque. In part, this is to full her obligation under High-Performance Computer Science Graduate Fellowship Program to spend three months as an intern at a DOE lab. But the next phase of Anne's research involves shared interests with Bill regarding the development of new algorithmic approaches for implementing search algorithms in a distributed computing environment. Bill has asked that we (Michael Lewis and Virginia Torczon) spend a week at Sandia, Albuquerque, at the start of Anne's internship, to discuss this new area of research and outline possible avenues for joint collaboration.

In addition, Tammy has asked us to spend a month at Sandia, Livermore, as part of an ongoing collaboration to develop pattern search/generating set search algorithms for handling general nonlinear constraints. During our visit to CSRI last summer, we finished the last of our revisions to an invited review paper on direct search methods for SIAM Review [9]. As part of this project, we undertook a thorough review of other recent work on direct search methods (e.g., [2, 3, 5, 18, 19, 20, 21]). From our review we see ways to combine a lot of these ideas with our own (e.g., [4, 7, 11, 12, 14, 15, 16, 17, 22]) to make pattern search even more flexible. The first result from this revisiting of current analysis for direct search was the definition of a new class of methods, which subsume pattern search, that we now call generating set search methods. With this revised perspective on handling nonlinear programming in the absence of reliable derivative information, last summer we drafted a paper on handling linear constraints for generating set search, which was submitted to SIAM Journal on Optimization [10]. The reviews have just come back and one of the goals at the start of our visit to Sandia, Livermore, will be to finish up revisions in light of the comments from the referees.

Algorithmic development
One outcome from our collaboration with Tammy last summer is that we now see a new way to use the linearly constrained methods to solve nonlinear constrained problems. The goal is to combine the results in [10] with work by Conn, Gould, Sartenaer, and Toint [1], to develop generating set search methods for nonlinear constraints. This is a further, and more flexible, generalization of the results in [17].

Software development
This year we are in an even better position to make progress on software development. Having finished all other Ph.D. candidacy requirements, this past year Anne Shepherd has actively pursued the development and implementation of pattern search for linearly constrained problems. She now has a working implementation that handles degenerate constraints. Anne has just begun the next step in her long-term plan, which is to develop effective parallel variants. Since some of the ideas she is pursuing dovetail nicely with work Bill Hart is doing on PICO and evolutionary optimization, the timing of our visit to Albuquerque is particularly apt. After several conversations with Bill, it is clear that we should work with Anne to write software tools that can be extended to some of Bill's algorithmic work outside the domain of pattern search.

Applications
The work undertaken during our visits to Sandia, Livermore is largely developmental in nature, but it has a practical impact on other work undertaken at Sandia. For instance, Tammy and Genetha Gray used prior results, as implemented in APPSPACK, in a collaboration with Kenneth Sale and Malin Young (both members of the Biosystems Research group at Sandia, Livermore), to examine the problem of transmembrane protein structure determination [6].

Further, after the collaboration of last summer, Tammy thoroughly revised APPSPACK [8]. Our understanding is that the new revised version of APPSPACK is now matching or besting all competition in the Community Problems and Solutions showdown being run by Tim Kelley, Department of Mathematics, North Carolina State University, as part of an NSF ITR project on sampling methods for optimization and control of subsurface flows (see http://www4.ncsu.edu/~ctk/community.html).

Another application includes optimization for circuit simulation using ChiliSpice and Xyce. In all these applications, a question that remains is how to deal effectively with constraints, which arise quite naturally in the definition of such application problems.

Participation
The proposal is that we first spend one week during the summer of 2004 at Sandia National Laboratories, Albuquerque, at the start of Anne Shepherd's three month summer internship. Our primary contact will be Bill Hart.

We then plan to spend one month during the summer of 2004 at Sandia National Laboratories, Livermore. Our primary contact will be Tammy Kolda.

Deliverables
This year we will deliver a prototype C/C++ implementation of a pattern search algorithm for linearly constrained optimization problems. The prototype implementation handles the case of degenerate constraints (which can occur in practice).

Impact
The success of pattern search has led to its incorporation in several software projects at Sandia National Laboratories, including OPT++, the DAKOTA software toolkit, and APPSPACK. Throughout the development of our software for handling constraints, we will continue to consult with all the parties who have already made use of our pattern search technology to ensure that any new software can be incorporated as quickly and easily as possible into their work and this can be applied as soon as possible to applications at Sandia National Laboratories.

Further, our work on pattern search now has been incorporated into the new Genetic Algorithms and Direct Search Toolkit for Matlab. The latest release handles linear constraints, but only when the constraints are nondegenerate. The MathWorks developer of this project, Rakesh Kumar, was greatly influenced by our earlier papers on pattern search and is very interested in incorporating the new software to handle degeneracy. He also is interested in further developments that allow the extension of pattern search to handle general constraints.

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Chapter 3. Sabbaticals

The following university faculty did all or part of a sabbatical stay at Sandia National Laboratories during calendar year 2004.

Dr. Rob H. Bisseling,
University of Utrecht

Max D. Gunzburger,
Florida State University

Dr. Fredrik Manne,
University of Bergen, Norway

Dr. James D. Teresco,
Williams College

Homer F. Walker,
Worcester Polytechnic Institute

Title: Partitioning and Combinatorial Scientific Computing

PI: Rob H. Bisseling, University of Utrecht

Dates: May 1, 2004 – July 23, 2004

CSRI POC: Bruce Hendrickson, (505) 845-7599

Project Summary:

Statement of participation
Funding is requested for a short-term sabbatical visit by Rob H. Bisseling, associate professor at the Mathematics Department of Utrecht University, The Netherlands, to the Computer Science Research Institute at the Sandia National Laboratories, location Albuquerque, NM. The period of the visit would be three months, starting sometime in April 2004. (Exact starting date to be determined later). The host would be Dr. Bruce Hendrickson.

My current research interests are:

- Combinatorial scientific computing, in particular partitioning methods for sparse matrices, based on hypergraph partitioning.
- Parallel multidimensional fast Fourier transforms.
- Models of parallel computation, in particular for communication load balancing.

The purpose of the visit is:

- To collaborate with Dr. Hendrickson and his colleagues in the Discrete Algorithms group, in particular Dr. Karen Devine, on improving hypergraph partitioning methods, both those developed and implemented by Vastenhouw and Bisseling in the package Mondriaan, and those developed by the Sandia team and implemented in the package Zoltan. It would be mutually beneficial to exchange ideas and perhaps to implement new features in these packages.
- To collaborate with Dr. Hendrickson on the application of partitioning methods for sparse matrices in new application areas, such as for instance information retrieval and bioinformatics, or other areas that are of importance to Sandia.
- To lecture at different US research institutes (including the Livermore location of Sandia, and also Old Dominion University, as a guest of Prof. Alex Pothen), on material from the book "Parallel Scientific Computation: A Structured Approach with BSP and MPI", by Rob H. Bisseling, Oxford University Press, February 2004. ISBN 0-19-852939-2. See http://www.oup.co.uk/isbn/0-19-852939-2.

Title: Report on accomplishments and contributions under contract number 18407 and plans for future participation in Sandia Laboratories projects

PI: Max D. Gunzburger, Florida State University

Dates: December 22, 2003 – September 30, 2004

CSRI POC: John Shadid, (505) 845-7876

Project Summary:

Report on accomplishments and contributions under contract number 18407 and plans for future participation in Sandia National Laboratories projects.

A list of projects in which I have been involved in under contract number 18407 is given below. The timeframe over which each project was carried out is given as are the participating Sandia personnel. A brief description of each project is provided. The level and nature of my participation up to now and in the future is indicated for each project. It is also highly probable that I will become involved in other Sandia projects in the future. Sandia has tons of interesting projects that I believe I can contribute to in meaningful ways; in fact, for me one of the great joys of visiting Sandia is the opportunity it affords me to learn about and contribute to a wide variety of very interesting projects.

Stabilized finite element methods
(T. Barth, P. Bochev, R. Lehoucq, and J. Shadid)
(Continuous work over 02 and 03 — Continuing in 04)
The regularization of finite element methods for linear and nonlinear convection-diffusion-reaction problems is a subject of great interest, mainly because such method are in widespread use, including within Sandia codes. However, there are settings in which these methods do not work well and others in which they are much misunderstood. We have been involved in a systematic study of various issues related to stabilized finite element methods. The most notable of these are described as follows.

Inf-sup stabilization of mixed finite element methods for the Stokes and Navier-Stokes equations
Finite element methods for the Stokes and Navier-Stokes equations based on the classical theory of mixed finite element methods require that the pressure and velocity finite element spaces satisfy the onerous inf-sup (or LBB) condition. This condition rules out, among other choices, equal order interpolation based on the same grid for the velocity and pressure. Not surprisingly, there has been much interest in the development of methods, collectively known as stabilized finite element methods, that circumvent the inf-sup condition. The result of this interest has been a plethora of methods proposed and analyzed, so many, in fact, that great confusion reigns over the relative merits of the methods and even about their proper definition. Clearing up this confusion is of practical importance because many researchers are using inferior methods when superior methods are just as easy to implement.

In [1], we systematically classified the many methods that have been previously developed and also some new methods we discovered by placing all the methods within a master template; each individual method can be derived from the template by appropriately choosing 2 integer-valued parameters. We also studied the accuracy of the methods and the performance of Krylov subspace iterative methods for the solution of the discrete systems. In this way we identified the best methods.

One result reported in [1] is that there seems to be a gap between the theoretical predicted performance of one class of methods and their performance observed in computations. In particular, existing theories predicted that this class of methods produced stable approximations only for a restricted set of stabilization parameters while computations showed that the methods are stable for any choice of that parameter. Understanding this gap is of significant practical importance because, other than the conditional stability property, this class of methods is superior to the other classes we identified in the taxonomy of [1]. We have developed a new method within this class and rigorously showed that it is indeed absolutely stable [2], i.e., that it is stable for any value of the penalization parameter.

I have been involved in this project as a full partner. There are still some issues to be addressed. In [2], we proved the absolute stability of a new method in the most practical class of methods, but we have not so far proved the absolute stability of the most popular method in that class; this property is indicated by computational experiments. This would be important to do because many practitioners are shying away from that method, despite its many desirable attributes, because of the erroneous belief that it is only conditionally stable. Thus, one of our goals for the upcoming year is to prove the stability of the existing method. We also want to undertake additional thorough computational studies of stabilized methods in the Stokes and Navier-Stokes equations settings to further refine knowledge about the relative merits of the many methods with respect to ease of implementation, efficiency, accuracy, and performance of iterative methods. (I should note that these goals remain from one year ago; they were temporarily put on hold as we pursued some other pressing issues.)

Stabilized finite element methods for advection-diffusion-reaction equations
We have considered the stability of pressure-Poisson stabilized finite element methods for transient flow problems. Here, stabilization is needed not only because of the incompressibility constraint, but also because of the small diffusion relative to the convection in practical problems. For reacting flows, one is often forced to use very small time steps in order to accurately resolve the reaction time scales. We have shown that conventional methods for deriving fully discrete, stabilized formulations introduce terms that can trigger instabilities for small time steps. These terms are engendered by the coupling between a consistently stabilized finite element discretization in space with a finite difference discretization in time. This coupling essentially introduces a dependence between the spatial grid size and the time step. We also illustrated our theoretical results through numerical examples that demonstrate the loss of stability. These results are reported in [8, 9]. We have continued our study into the sources of instability by closely studying the algebraic properties of the discrete system. This work will be reported on in [7].

Now that we have identified the stability problem of conventional methods, we are in the process of developing stable methods based on space-time finite element discretizations. Some very preliminary work shows that this approach has great promise because it fully accounts for the transient nature of the problem. We will be developing, implementing, and testing the new methods in the near future.

Hierarchical finite element methods for compressible flows
(M. Calhoun-Lopez and C. Ober)
(Continuous work over 02 and 03 — Possibly continuing in 04)
Finite element methods possess several advantageous features that have made them the methods of choice in many if not most applications. However, despite these advantages, finite element methods have not been widely adopted and have certainly not supplanted finite volume methods in the compressible flow community. On the other hand, because of the potential advantages they offer, finite element methods for compressible flows have been a subject continuing interest. In recent years, some finite element methods, e.g., discontinuous Galerkin methods, have emerged that have begun to fulfill the potential advantages of finite element methods. However, these methods have several disadvantages as well, not the least of which is that they involve many more degrees of freedom that one would expect to need.

We have been studying a new class of methods, based on hierarchical finite element bases, for inviscid, compressible flow problems. Hierarchical bases differ from the standard, locally supported bases, in that they are built up from coarse grids to fine grids by keeping the basis function on the coarser grids and only adding at each grid level the basis functions that are needed to span the resulting finite element space. The big advantage of hierarchical bases is that, unlike standard bases, they are multiscale in nature, i.e., they contain low, medium, and high (relative to the finest grid) frequency functions. Seemingly the big disadvantage of hierarchical bases are that they are not locally supported. Fortunately, it has been shown that one can efficiently change from standard to hierarchical bases and back through simple, very sparse matrix operations so that in practice, this disadvantage does not have any import.

The big advantage of hierarchical finite element bases, i.e., their multiscale nature, allows for the selective application of artificial diffusion to only the high frequency components of approximate solutions. This approach was pioneered in the context of spectral methods (where the multiscale nature of bases is natural)

by E. Tadmor and co-workers. Such selective application of diffusion is not possible in the context of finite volume and standard finite element methods. Being able to apply it to finite element methods by using hierarchical bases is important because spectral methods are not as flexible, e.g., with respect to geometries, as are finite element methods.

We have implemented piecewise linear and quadratic hierarchical finite element methods with selective high frequency artificial viscosity application to one- and two-dimensional scalar and vector conservation laws. The results are very promising (with respect to the quality of approximate solutions) and have served to identify several potentially important advantages of our approach over both finite volume and spectral methods. For example, our methodology can easily and very cheaply identify the location of discontinuities. This may results in inexpensive and effective methodologies for adaptive gridding and for the selective application of artificial diffusion only in the vicinity of discontinuities. As a result, more efficient and more accurate methods may be developable. We are in the final stages of preparing a paper [13] that contains mostly theoretical results about our method, e.g., rigorous convergence proofs, and are also well along the preparation of another paper [14] that focuses on algorithmic and implementation issues and extensive computational tests.

I have been a full partner in this project. I was the major professor for M. Calhoun-Lopez who was in residence at Sandia last year and who completed his Ph.D. studies at Iowa State University last summer.
The hierarchical finite element for compressible flows project is the subject of Calhoun-Lopez's dissertation [12]. Marcus is now a postdoctoral associate at the Center for Scientific Computation and Mathematical Modeling at the University of Maryland which is directed by Professor Eitan Tadmor, one of the leading figures in the numerical solution of hyperbolic conservation laws. Professor Tadmor has, in fact, expressed great interest in Marcus' work and will be getting involved in the further development of the methods Marcus and I have devised. Over the next year, Marcus will incorporate the hierarchical finite element capability into existing Sandia codes. Although I intend to keep working on this method class, involvement with Sandia will depend on the level of interest that Sandia personnel, e.g., Dr. C. Ober and others, have in the further development of our methodology.

Least-squares finite element methods
(P. Bochev)
(Continuous work over 02 and 03 — Continuing in 04)
For over a decade, Pavel Bochev and I have been very involved in the development, analysis, and implementation of least-square finite element methods for the solution of problems governed by partial differential equations. Out joint work on this class of methods during the 2002 and 2003 fiscal years has focused on two directions.

Optimization and control problems
Optimization and control problems for systems governed by partial differential equations have been, in many applications, a subject of interest to experimentalists, theoreticians, and computationalists. Most of the efforts in the latter direction have employed elementary optimization strategies. More recently, mathematicians, scientists, and engineers have turned to the application of sophisticated optimization strategies for solving optimization and control problems for systems governed by partial differential equations. Today, many different local and global optimization strategies, e.g., Lagrange multiplier methods, sensitivity or adjoint-based gradient methods, quasi-Newton methods, evolutionary algorithms, etc., are in common use.

Several popular approaches to solving such optimization and control problems for systems governed by partial differential equations are based, one way or another, on optimality systems deduced from the application of the Lagrange multiplier rule. This may not be surprising since the Lagrange multiplier rule is, of course, a standard approach to solving finite-dimensional optimization problems. Perhaps more surprising is that penalty methods, which are another popular approach for the latter setting, have not engendered anywhere near as much interest for the infinite-dimensional problems which are of interest here. We have shown why naively defined penalty methods may not be practical and, using methodologies associated with modern least-squares finite element methods, we showed how practical penalty methods

can be defined. Moreover, we showed that penalty methods offer certain efficiency-related advantages compared to methods based on the Lagrange multiplier rule. Our results, in the context of the Stokes equations, were reported in [3]. Results in more general settings are to be reported on in [5, 6].

I have been a full partner in this effort. So far, our studies have been mostly of a theoretical nature; this was a necessary first step towards placing our algorithms on a firm foundation. We may continue this study by implementing the algorithms we have devised and testing them on standard optimization problems for partial differential equations. One important practical question we have to address is the effect of the penalty parameter on the conditioning of the discrete system; we will examine this question by both analytical and computational means.

Relating least-squares and mixed finite element methods
Least-square finite element methods provide an attractive alternative to mixed-Galerkin finite element methods for many problems for which the latter class of problems require the satisfaction of onerous compatibility conditions. In formulating a least-squares finite element method for a specific problem, or for a class of problems, one has many choices available that can affect the accuracy, stability, efficiency, and robustness of the resulting method. We have, in the past, contributed a great deal to the understanding of how these choices should be made. Recently, we have uncovered a deep connection between least-squares finite element methods and primal/dual pairs of mixed finite element methods which allowed us to define least-squares finite element methods that are, in some sense, "optimal." For example, using these connections, we have been able to solve one of the remaining theoretical issues connected with least-squares finite element methods for the Poisson equation, namely obtaining optimal L2-norm error estimates for all variables. This work was reported in [4].

Further studies along these lines will address other systems, e.g., linear elasticity. In addition, it is likely that Pavel's and my research program into least-squares finite element methods will continue to address several other outstanding issues.

Hypercube sampling and its applications
(V. Romero)
(Continuous work over 02 and 03 — Continuing in 04)
Uniform sampling in high-dimensional hypercubes forms the basis of several stochastic and deterministic algorithms, e.g., numerical integration and stochastic optimization. Many improvements over the classic Monte Carlo approach have been suggested, including Latin hypercube, distributed hypercube, Halton sequence, and Hammersley sequence sampling. For many years, I have been involved in the development of centroidal Voronoi tessellations (CVT's) as, among many other things, a means for obtaining high-quality uniform point distributions. CVT's are special Voronoi tessellations of a region for which the generators of the Voronoi diagram are also the centers of mass, with respect to a given density function, of the corresponding Voronoi cells. I have also been involved in the development of very fast, scalable, probabilistic algorithms for constructing CVT's. Two of the applications of the CVT methodology that I have helped develop are to grid generation and point placement for meshless and particle methods; in these contexts, CVT point placement have proven superior to all known point placement strategies for determining uniformly distributed points in general regions. Thus, it was natural to study CVT point placement strategies for uniform sampling in hypercubes. We have compared CVT-based point sampling strategies with many other uniform hypercube point sampling strategies. With respect to several volumetric measures of uniformity, the CVT point sampling strategy has proven to be vastly superior to all known sampling strategies. However, CVT point samples are inferior with respect to the uniformity of their projections onto lower-dimensional faces of the hypercube; this property is important in some applications. For such applications, we have developed a variant of CVT-based point sampling that possesses the Latin hypercube property and thus has very good projections onto lower-dimensional faces. These Latinized-CVT point samples are still substantially superior, with respect to volumetric measures of uniformity, when compared to other LHS methods as well as to standard quasi-Monte Carlo sequence methods.

CVT point sampling, however, may be even more useful in other settings. For example, in many applications, one wants points that are nonuniformly distributed according to a prescribed distribution function. Most existing methods can only produce quasi-uniformly distributed samples; to get a

nonuniformly distributed sample, inverse transformation with respect to the distribution function must be carried out. For all but the simplest distribution functions, this can be an expensive proposition. CVT methodologies, on the other hand, can directly produce nonuniform point samples at almost the same costs as uniform samples. Moreover, CVT point sampling can just as easily handle general regions as it does hypercubes, and lends itself well to adaptive and hierarchical point sampling.

I am a full partner in this effort. Our work has resulted in several papers [11, 15, 16]. We plan to continue to work on this project, addressing the many applications of hypercube point sampling and more difficult problems that will further highlight the advantages of CVT point sampling techniques.

Electromagnetic inverse problems in geophysics
(P. Bochev, D. Day, G. Newman, and R. Tuminaro)
(Almost no involvement in 03; potential involvement in 04)
The listed Sandia personnel have embarked on an ambitious project aimed at developing a methodology and related software for the solution of electromagnetic inverse problems applicable to, e.g., the identification of material properties. The project has several aspects including, in the initial stages, the development and application of better discretization methods and better solvers. So far, my involvement in the projects has been totally peripheral. My more full involvement awaits the completion of the initial stage of the project. At that point, it is likely that I will be able to contribute to two aspects of the project. First, there already has been developed and implemented a least-squares based optimization method for parameter identification in which the parameters are allowed to vary on the scale of the discretization grid. It is planned to use the output of this software as input for a sophisticated shape optimization approach to obtaining better interfaces between materials and better estimates of material properties. It will be probably be very desirable to smooth, i.e., denoise, the sometimes rough output of the least-squares based optimization step; otherwise, any shape optimizer may have trouble converging. For this purpose, I have previously developed an image segmentation method that is effective and inexpensive and produces sharp, denoised interfaces. This method may be applicable to the transfer of output from the least-squares based optimization step to the shape optimization step. For some time now, I have also been interested in shape optimization so that I may be able to contribute to the development of this aspect of the project as well.

Papers prepared under Sandia contract 18407
[1] T. Barth, P. Bochev, M. Gunzburger, and J. Shadid; A taxonomy of consistently stabilized finite element methods for the Stokes problem; accepted by SIAM J. Sci. Comput.
[2] P. Bochev and M. Gunzburger; An absolutely stable pressure-Poisson stabilized finite element method for the Stokes equations; accepted by SIAM J. Numer. Anal.
[3] P. Bochev and M. Gunzburger; Least-squares finite element methods for optimization and control problems for the Stokes equations; accepted by Comp. Math. Appl..
[4] P. Bochev and M. Gunzburger; On least-squares finite element methods for the Poisson equation and their connection to the Dirichlet and Kelvin principles, submitted to SIAM J. Numer. Anal.
[5] P. Bochev and M. Gunzburger; Least-squares finite element methods for optimization and control problems I: Lagrange multiplier formulations; in preparation.
[6] P. Bochev and M. Gunzburger; Least-squares finite element methods for optimization and control problems II: Penalty formulations; in preparation.
[7] P. Bochev, M. Gunzburger, and R. Lehoucq; On stabilized finite element methods for the Stokes problem in the small time-step limit, in preparation.
[8] P. Bochev, M. Gunzburger, and J. Shadid; On stabilized finite element methods for transient problems with varying time scales; Fifth World Congress on Computational Mechanics, (CD-ROM), International Association for Computational Mechanics, Vienna, 2002.
[9] P. Bochev, M. Gunzburger, and J. Shadid; On inf-sup stabilized finite element methods for transient problems; accepted by Comp. Meth. Appl. Mech. Engrg.
[10] P. Bochev, M. Gunzburger, and J. Shadid; Stability and streamline upwind Petrov-Galerkin (SUPG) finite elements for transient advection-diffusion problems; submitted to Comp. Meth. Appl. Mech. Engrg.
[11] J. Burkardt, M. Gunzburger, J. Peterson, and Y. Saka; Improved hypercube point sampling including improved LHS designs; in preparation.

[12] M. Calhoun-Lopez; Numerical solutions of hyperbolic conservation laws: Incorporating multiresolution viscosity methods into the finite element framework; Ph.D. Theses, Department of Mathematics, Iowa State University, Ames, 2003.
[13] M. Calhoun-Lopez and M. Gunzburger; A finite element, multi-resolution viscosity method for hyperbolic conservation laws; to be submitted by the end of the year to the SIAM J. Numer. Anal.
[14] M. Calhoun-Lopez and M. Gunzburger; Implementation and testing of a finite element, multiresolution viscosity method for hyperbolic conservation laws; in preparation.
[15] V. Romero, J. Burkardt, M. Gunzburger, J. Peterson, and K. Krishnamurthy; Initial application and evaluation of a promising new sampling method for response surface generation: Centroidal Voronoi tessellations; submitted.
[16] V. Romero, J. Burkardt, M. Gunzburger, and J. Peterson; Initial evaluation of centroidal Voronoi tessellation method for statistical sampling and function integration; submitted.

Title: Graph Coloring in Optimization

PI: Fredrik Manne, University of Bergen, Norway

Dates: August 2004 – June 2005

CSRI POC: Bruce Hendrickson, (505) 845-7599

Project Summary:

With this I apply to spend my sabbatical term for the academic year 2004-2005 at CSRI, Sandia National Laboratories. The following document gives a closer description of my background and the research I intend to perform while at CSRI.

Background
I am employed as a professor at the Department of Informatics, University of Bergen, Norway. This is a position I have held for the last 6 years, the last 3 years as vice chairman of the department. My primary research interests include Combinatorial Scientific Computing, graph algorithms, parallel algorithms, and distributed computing.

Current Research
My research is focused on discrete algorithms in large scale applications, a field known as "Combinatorial Scientific Computing". Within this field I have worked with parallelizing various linear algebra codes, load balancing on parallel computers, and developing parallel algorithms for graph coloring. Lately, I have also worked on distributed algorithms.

My research spans from practical implementations on state of the art super computers to more theoretical computer science, particularly algorithm development and analysis.

Within the field of graph coloring I have together with my former student A. Gebremedhin developed the first greedy truly scalable parallel graph coloring algorithm.

The Graph coloring problem (GCP) consists of assigning as few colors as possible to nodes in a graph such that two adjacent nodes are assigned different colors. The GCP arises in a number of scientific computing and engineering applications such as parallel numerical computations, optimization, time tabling and scheduling and frequency assignment.

In a parallel application a graph coloring is usually performed in order to partition the work associated with the nodes into independent subtasks such that the subtasks can be performed concurrently. The underlying assumption being that the nodes represent tasks and that the edges are dependencies among these. The tasks with nodes that have the same color will then make up an independent set that can be performed concurrently. One example of this is in parallel adaptive mesh refinement where a graph coloring can be used to determine independent sets of triangles that can be refined simultaneously without interfering with each other.

In numerical optimization graph coloring is used to minimize the number of function evaluations needed to compute Jacobian and Hessian matrices via finite differences or though automatic differentiation.

There exists several linear, or close to linear, time greedy coloring heuristics that have been shown to produce colorings of high quality. Even though these algorithms are fast they can on very large or distributed data sets still be costly to evaluate. For this purpose it is desirable to develop fast parallel and/or distributed algorithms to solve the GCP. Previous efforts have lead to parallel algorithms that allows the graph to remain distributed while the coloring is computed. Unfortunately, these algorithms did not give a reduced execution time as the number of processors were increased.

Our *shared memory* algorithm was the first algorithm for the GCP that achieved speed-up as the number of processors were increased. The algorithm is based on letting each processor color its portion of the graph independently of what the other processors are currently doing. As this might lead to an inconsistent coloring a second stage is used to detect any conflicts which are then later corrected.

Our initial motivation for working on this problem was to speed up a parallel eigenvalue computation. Later collaboration with Alex Pothen from The Old Dominion University has led to applications of this work in the area of numerical optimization methods to compute Jacobian and Hessian matrices. In this setting one uses function evaluations to determine rows or columns (or rows) using one function evaluation if the desired columns are structurally orthogonal. This is important to exploit as the function evaluations can be costly. Partitioning the columns into the minimum number of groups such that each group can be evaluated with one function evaluation reduces to a graph coloring problem. In this setting the notion of "neighbor" is somewhat more general than for the traditional problem and depending on the type of matrix one wish to compute one might have to take into account nodes further away than just the closest neighbors. Theoretical and experimental results have shown that our algorithm can be modified to handle these conditions well.

As a continuation of my work on parallel algorithms I have lately also started to work on distributed algorithms. My main interest concerns "self -stabilizing" algorithms. These are distributed algorithms that run on a set of mobile units that try to solve some common problem without the use of a central command. Each unit can only "see" and communicate with its nearest neighbors. The combined effort of all the units should together be able to come up with a global solution to a given problem without any particular unit having complete knowledge of the structure of the entire system. In addition, if the configuration changes due to movement or malfunctioning among the participants the solution should also change to reflect this. Applications of these types of algorithms can be found in various mobile ad-hoc networks. This could for instance be for maintaining a communication network among autonomous robots in a hostile environment or as a general purpose network without base stations. My research in this area has been performed in close cooperation with Jean Blair from The United States Military Academy at West Point. As of 2004 I have received a grant from the Norwegian Research Council for a project to study frequency allocation problems in these types of networks. This is again closely related to my work on parallel graph coloring algorithms.

I have also been working on a project with the goal of computing exact or lower bounds on the minimum amount of fill in grid graphs when performing sparse factorization. The purpose of this work is to establish bounds for a number of test cases such that one can compare the quality of existing software for reordering sparse matrices. So far this has turned out to be a very difficult problem and we have only been able to come up with exact lower bounds for relatively small instances.

Research Plan

It is my wish to come to CSRI to continue my work on parallel graph coloring in close collaboration with the researchers at CSRI. CSRI has expertise on the types of applications such as the Zoltan project and ASCI simulation codes, where this work can have an impact. In particular, the current version of the parallel graph coloring algorithm has as previously mentioned so far only been implemented on shared memory parallel computers. It is my intention to develop and test a *distributed memory* version of this algorithm. This is an important step in making the algorithm more useful to others as nearly all of the Sandia codes that could make use of a parallel graph coloring algorithm are themselves implemented on distributed memory platforms.

There are several issues involved in developing such a code. One of these is that on a shared memory computer each processor has direct access to the colors that the other processors have assigned so far, but on a traditional distributed memory computer using the MPI-1 message passing library for communication this information would have to be requested and sent back explicitly thus requiring the processors to synchronize which would slow down the computation. There is also a possible danger of flooding the recipient with requests that it is not yet ready to process. A more desirable solution would be to use explicit non-intrusive "get" commands to fetch information from the other processors without them having to directly participate in the exchange of data. These types of commands are now available through the

message passing library MPI-2. However, this needs to be tested and MPI-2 has still not been implemented on all platforms that support MPI-1.

I also intend to continue the work on computing lower bounds for the amount of fill in grids graphs making use of the extensive knowledge about algorithms for sparse reordering at CSRI.

Although I am not aware of any research at CSRI (or Sandia Labs in general) related to self-stabilizing algorithms I plan to continue this work partly in cooperation with Jared Saia from the University of New Mexico.

Contacts within CSRI and UNM

I have had regular contacts with Erik Boman and Bruce Hendrickson the last couple of years. During "SIAM 50th Anniversary and 2002 annual meeting" in Philadelphia Hendrickson and Alex Pothen invited me to give a talk on "Parallel algorithms for distance-2 graph coloring". During the spring of 2003 I visited CSRI for three days to prepare for spending my sabbatical there. I had discussions with several researchers about possible future research projects and also gave a talk about my own research. The most concrete outcome of this were discussions with Karen Devine about developing a parallel graph coloring algorithm for distributed memory and merging this with Zoltan. One possible application might then to be parallelize the hypergraph partitioner currently under development in Zoltan.

While I was in Albuquerque I also visited The Department of Computer Science at The University of New Mexico where I had talks with Professor Jared Saia bout common interest within the field of distributed algorithms. I also talked with the department chairman Professor Deepak Kapur about spending part of my sabbatical at the University of New Mexico. As a consequence I have since received a letter of invitation from Dr. Kapur inviting me to do so.

Another connection with Sandia concerns work that I did some years ago on efficient load balancing algorithms that has since been continued by Ali Pinar who was a student of Bruce Hendrickson and by Johan Steensland who is now a post. doc. at Sandia Labs in Livermore.

Title:	Dynamic Load Balancing for Parallel Adaptive Scientific Computation
PI:	James D. Teresco, Williams College
Investigator:	Luis Gervasio and Jamal Faik, Williams College
Dates:	September 2003 – Summer 2004
CSRI POC:	Karen Devine, (505) 845-7585

Project Summary:

I would like to propose a visit to the Computer Science Research Institute at Sandia National Laboratories in Albuquerque during the fall of 2003. I have been part of a successful collaboration between Joe Flaherty's group at Rensselaer Polytechnic Institute and Karen Devine and others in Sandia's Zoltan group for a number of years. I believe that my spending some time at Sandia this fall would be beneficial to all of us.

I will be on leave from my teaching duties at Williams College. My arrangement with Williams is that the College pays my full salary in one semester and half in the other. I would like to visit from late August until late November 2003. If the proposed visit is as successful and productive as I expect, I may pursue a second visit to Sandia in the spring or summer of 2004. Ideally, two Rensselaer graduate students who have been involved in our collaboration, Luis Gervasio and Jamal Faik, would be able to visit Sandia as well for all or part of my visit. We intend to arrange this separately from this proposal.

1 Research Background

My research interests are in dynamic load balancing for parallel adaptive scientific computation. In particular, I am interested in dynamic load balancing when the target computer systems are heterogeneous and/or hierarchical, and for highly adaptive problems.

Target parallel environments for modern, adaptive scientific computation range from the largest tightly-coupled supercomputers to heterogeneous clusters of workstations, with a variety of processor, memory, and communication hierarchies. Hierarchical and heterogeneous systems are increasingly common, a trend that is likely to continue with the increasing popularity of clusters of multiprocessors and the emergence of grid technologies, or metacomputing. This presents challenges for the development of efficient software, particularly influencing dynamic load balancing procedures. Whereas partitioning for a flat network with uniform processing nodes involves the determination of partitions of equal size and minimal boundary, optimal partitioning in other environments must consider the heterogeneity and hierarchy of processors, networks, and memories.

I have been investigating procedures for optimal task scheduling and dynamic load balancing in these nonuniform computational environments. I began this work by developing the Rensselaer partition model (RPM) [11] as part of my dissertation. Original RPM development was concerned with supporting the Meshing Environment for Geometry-based Analysis (MEGA) [10] and the Trellis framework [1]. RPM has also been used as the foundation of the parallel version of the Algorithm-Oriented Mesh Database (AOMD) [9]. The software interfaces with Sandia's Zoltan library [4] for dynamic load balancing.

My recent work on system-sensitive dynamic load balancing involves the design and implementation of a persistent and dynamic machine model for use with Zoltan, which incorporates relative capabilities of the composing blocks of the execution environment. The model has a tree structure that can easily be traversed by balancing procedures through a general interface that allows a topology-driven, yet transparent, execution of hierarchical partitioning. Each node in the tree contains its relative computing power and percentage of load. These capabilities are assessed initially by running a benchmark program and are updated dynamically by agents, threads that independently monitor the performance of each node while the user application is running. Processing nodes at the leaves of the tree have data representing the relative computing power of their processors. Network nodes have a bandwidth property and an aggregate

computing power calculated as a function of the powers of their children and the network characteristics (e.g., bandwidth and latency). For load balancing purposes, we interpret a node's power, once normalized, as the percent of the load of its immediate parent that it should be assigned, based on its communication and computational capabilities. These relative “power" values can be used with any procedure that can produce variable-size partitions.

Preliminary results have shown significant benefit to this approach. We solve a two-dimensional Rayleigh-Taylor instability problem on a rectangular domain using eight processors of the Sun cluster at Williams College: five 450MHz Sparc UltraII processors, and three 300MHz Sparc UltraII processors, connected by fast (100 Mbit) Ethernet. Given an equal distribution of work, the fast nodes will be idle 1/3 of the time waiting for the slow nodes to complete their work. By giving 50% more work (as determined by the benchmarks) to each of the five fast nodes, an overall speedup of 24% is possible. We achieve a total wall clock time (including setup and all computation and communication) reduction from 3396 seconds to 2912 seconds, an improvement of 14.25%. We expect that the improvement in the actual computation time is much closer to the 24% theoretical maximum. Similar tests using the dynamic monitoring capabilities are underway. I have also been heavily involved in work on Zoltan's Octree/SFC partitioning procedure. Since an octree is easily constructed from an arbitrary mesh, the procedure is independent of any octree procedures that are used for mesh generation or adaptive refinement. Partitioning may be done in parallel [5, 6] by distributing the tree across the participating processors. Gervasio [7] developed the Octree/SFC partitioning procedure within Zoltan and studied traversals of the octree by space-filling curves (SFCs) corresponding to Morton, Hilbert, and Gray code orderings. The Hilbert ordering generally achieves the best partitions of the three orderings, which likely results from the greater locality of the Hilbert curve [3]. Campbell [2, 3] redesigned the SFC implementation to provide better efficiency, scalability, and extensibility. Gervasio has modified the Octree/SFC procedure to compute non-uniform partition sizes, to allow its use for system-sensitive load balancing experiments. Our continued interest in the Octree/SFC and other SFC-based partitioning and load-balancing procedures is motivated by their incremental nature. For highly-adaptive problems where dynamic load balancing is needed frequently, incremental procedures provide the necessary speed and limited data migration to allow for efficient rebalancing.

2 Proposed Research

During a visit to Sandia, I would continue work on both system-sensitive load balancing and on the Octree/SFC procedure. Working closely with the Zoltan group will help us to perform the proposed research more quickly, and will allow us to find new and interesting projects of mutual interest.

2.1 System-sensitive Balancing

- We will conduct a study to test our system-sensitive balancing procedures on a variety of heterogeneous and hierarchical systems of interest. We have worked primarily on a cluster of Sun servers and workstations at Williams College. We will test the current benchmarking and dynamic monitoring approach on other systems available at Sandia, Williams, Rensselaer, and elsewhere.
- Our current node power estimates take into account relative processor speeds and network capabilities. We would like to extend this model, including the dynamic monitoring agents, to include memory availability. A process that begins to use virtual memory often incurs unacceptable time penalties. We will place a threshold on the amount of work that can be assigned to one process based on its available main memory.
- We will use the machine model to guide a hierarchical load balancing procedure, to achieve partitions that use different algorithms or parameters, as appropriate, at different levels of the machine model hierarchy. Automating this requires that each Zoltan balancing procedure be able to produce numbers of partitions not equal to the number of processes. Such hierarchical balancing has the potential for benefit on any hierarchical system, but will become essential if distributed cluster architectures are to be utilized. Consider an adaptive computation on two clusters, connected by a campus-area network or even a wide-area network. These computations are enabled by grid tools such as MPICH-G2 [8]. Here, it is essential to minimize communication across the slow network interface. We intend to investigate the use of hierarchical balancing in this extreme situation.

- We plan to conduct a thorough analysis of the performance of Zoltan's load balancers. The studies will examine running time, load balancing accuracy, partition quality statistics such as surface indices (surface-to-volume ratios) and interprocess adjacencies, as well as incrementality, for real adaptive solution processes.

A preliminary study was conducted in 2002 [12]. Such information will be generally useful to Zoltan users, who could make better informed decisions when choosing from among Zoltan's procedures. It is of particular interest to the development of system-sensitive balancers that choose automatically from among the available procedures, based, at least in part, on their performance on the target architecture. We intend to include (i) a more thorough set of available procedures and parameters (HSFC, BSFC, Octree/SFC, more options of Jostle and Parmetis), (ii) a variety of computer systems (Sun cluster, PC clusters with different interconnects, networks of workstations, IBM SP and other ASCI-class supercomputers, metacomputers), (iii) a variety of applications (two- and three-dimensional simulations, highly adaptive, applications of interest to Sandia), and (iv) a variety of mesh structures (different element types, both simple and complex geometries and adaptive behavior).

2.2 Octree/SFC Procedure

For the Octree/SFC procedure, efficiency improvements and a detailed incrementality study are planned.

- We will consider a more adaptive approach to tree construction for the Octree/SFC procedure. The tree structure is already adaptive to the extent that a leaf octant is only refined if an object is inserted that overfills that octant, resulting in a deeper (more refined) tree in areas where objects are concentrated. However, we propose to take an approach similar to that taken by Zoltan's HSFC and BSFC algorithms and recursively refine only those octants that lie at partition boundaries until a satisfactory load balance is achieved. The startup cost of Octree/SFC would be reduced, yet the same partitions would be produced.
- As part of the performance comparisons described in the previous section, we will study the incrementality of Octree/SFC and other Zoltan procedures. A fast, incremental procedure is essential when solving highly adaptive problems. We will measure running times and the amount of data moved during load balancing in response to small changes in the mesh.
- We believe that Octree/SFC and other procedures in Zoltan can benefit from knowledge retained across successive load balancing invocations. While startup costs are often small relative to repartitioning and migration costs, we expect that startup costs will be more significant when highly-adaptive, terascale problems are being solved. Reconstruction of the octree (or analogous internal structures used by other Zoltan procedures) and reinsertion of all objects when only a fraction of these objects have changed requires work on the order of the total number of objects rather than the total number of objects that have changed. For Octree/SFC, this would require the fully-maintained tree structure, previously implemented by Campbell [2]. It would also require that objects' global Zoltan identifiers be consistent across calls. If an application can guarantee this, and it calls Zoltan functions to allow the update of the tree or other intermediate data structures when the collection of objects is modified, a truly dynamic and scalable repartitioning could be achieved. Similar approaches could benefit other Zoltan procedures that use intermediate structures to compute the partitions.

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Title: Robust nonlinear solution algorithms for large-scale complex coupled nonlinear PDE systems

PI: Homer F. Walker, Professor, Worcester Polytechnic Institute

Dates: September 2003 – May 2004

CSRI POC: John Shadid, (505) 845-7876 and Roger Pawlowski, (505) 284-3740

Project Summary:

I am requesting support to visit Sandia National Laboratories in Albuquerque during my sabbatical from Worcester Polytechnic Institute in the 2003-2004 academic year. The specific proposal is to visit for nine two-week periods (one per month) from September 2003 through May 2004. During these visits and also the interim periods, I will pursue joint research with collaborators at SNL.

A major research activity during the sabbatical will be to advance and extend current work with John Shadid, Roger Pawlowski and others on robust nonlinear solution algorithms for large-scale complex coupled nonlinear PDE systems. This research will continue our current investigation of globalizations of inexact Newton methods applied to steady-state problems, with further development and study of linesearch and trust-region methods, and will also include consideration of new possibilities, such as nonlinear preconditioning (domain-based and multigrid), that may enhance robustness. We will also investigate extensions of Newton's method that use higher-order information, such as tensor methods. Broad application categories are likely to be (1) transport reactions systems with low heat release, such as fluid flow, CVD, and biological cell modeling, and (2) transport reactions systems with high heat release, such as combustion and catalytic reactors. The overall goal will be to develop methods and implementations that are robust and efficient when applied to these problems on massively parallel computers.

I will also explore opportunities for research in new areas with other investigators. Possibilities at present include working with (1) Scott Hutchinson and others on the Xyce team to explore nonlinear solvers and homotopy/continuation methods that exploit special structure in coupled device-circuit systems, (2) Andrew Salinger and others involved in Loca development to investigate linear and nonlinear solution methods in continuation and bifurcation algorithms, and (3) Rich Lehoucq, David Day, Teri Barth, and others to collaborate on eigensolvers and iterative linear algebra methods.

Chapter 4. Workshops/Sponsorships

The following workshops were either hosted by the CSRI or partially supported by the CSRI during 2004.

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1) SIAM Workshop on Combinatorial Scientific Computing – February 27-28, 2004 – Hendrickson

2) Eight Copper Mountain Conference on Iterative Methods – March 28-April 2, 2004 – Tuminaro

3) Fifth International Conference on Linux Clusters – May 17-20, 2004 – Brightwell and Pundit

4) Second Sandia Workshop on PDE-Constrained Optimization "Toward Real-time and Online PDE-constrained Optimization" – May 19-21, 2004 – Bart van Bloemen Waanders

5) Proposal for CSRI Workshop on Numerical Aspects of Circuit and Device Modeling (NACDM) – June 23-25, 2005 – Keiter

6) Proposal for CSRI Workshop on Multiscale Mathematics – December 13-15, 2004 – Lehoucq and Collis

Title: SIAM Workshop on Combinatorial Scientific Computing

PI: Bruce Hendrickson

Dates: February 27-28, 2004

CSRI POC: Bruce Hendrickson, (505) 845-7599

Project Summary:

I am requesting that the CSRI provide some funding to support the upcoming SIAM Workshop on Combinatorial Scientific Computing. This will be the first meeting of its kind, and will occur February 27th and 28th in San Francisco, immediately following the SIAM Conference on Parallel Processing. More information about the workshop can be found at www.siam.org/meetings/pp04/cscworkshop.htm, including the following rationale.

"Combinatorial algorithms and mathematics are a critical enabling technology for scientific computing, especially for large-scale problems and high-performance computers. Combinatorial techniques are employed in sparse direct solvers, parallel computation of irregular problems, computational solution of partial differential equations, iterative linear equation solvers such as domain decomposition and algebraic multigrid, preconditioners for iterative linear solvers, mathematical programming, numerical optimization, automatic differentiation, computational biology, etc. Combinatorial techniques that have been applied to scientific computing problems include graph and hypergraph models of problems, path structures in undirected and directed graphs, matchings, colorings, network flows, matroids, graph embeddings, independent sets, spectral graph theory, etc. Geometric and probabilistic computing are closely related areas that we include under the rubric of combinatorial methods.

Researchers developing and applying combinatorial mathematics and algorithms in different areas of scientific computing have a great deal of overlap in their interests, mathematical aesthetics, objectives, and tools. Unfortunately, in usual taxonomies of scientific computing, these application areas form widely scattered research sub-communities. As a consequence, combinatorial algorithms researchers in these sub-communities tend to be isolated and unaware of the broader sets of problems, techniques, and researchers. This lack of contact leads to duplication of effort and slows research progress. It is also an impediment to young researchers since the sub-communities are too small to support their professional development as researchers in applied combinatorics.

To address these needs, the community of researchers working in combinatorial algorithms in scientific computing has organized for the past 18 months under the banner of Combinatorial Scientific Computing (CSC). A list serve has been established at http://list.odu.edu/listinfo/csc, and minisymposia have been organized at a number of meetings including the past two SIAM annual meetings, ICIAM, SIAM-CSE, and SIAM PP04. This workshop, CSC04, is the next step in building the CSC community."

As you know, Sandia has a long history of leading work in the application of discrete algorithms to scientific computing. I personally feel that this is a distinguishing strength of our capabilities in high performance computing. By helping to ensure the success of CSC04, Sandia would be continuing to demonstrate leadership in this important area, and also ensuring the success of founding meeting underlying the emerging discipline. It is worth noting that the idea for nurturing a community around the unifying theme of combinatorial scientific computing came out of Alex Pothen's sabbatical visit to Sandia.

SIAM has a proposal to Chuck Romine to provide $10K of funding for this workshop, the majority of which will be used to pay for student travel. After consultation with SIAM, I am asking for an additional $4325K of CSRI funding to cover the following expenses.

Title: Eighth Copper Mountain Conference on Iterative Methods

PI: Ray Tuminaro

Dates: March 28-April 2, 2004

CSRI POC: Ray Tuminaro, (925) 294-2564

Project Summary:

This workshop is the premier U.S. forum for the presentation of original research in the development of scalable iterative solutions of very large linear systems. Sandia ASCI projects rely very heavily on iterative solvers technology. Each year a large number of Sandians attend this meeting. If this meeting were not held future research by Sandia staff might be compromised by not being able to benefit from research presented at this conference. The Copper Mountain Iterative Methods Conference also provides an excellent opportunity to recruit high-quality applications for both visitors, summer students and future staff. The meeting is held in high regard by some of our funding sources such as the MICS program office (who attend the meeting as well). It is very important that Sandia have a good presence at this meeting. Sandia's contributions help keep registration fees low which encourage broad participation including active academic and student involvement. It also helps directly pay for crucial student support so that young people who might not be able to partake in the meeting can attend and present.

The contribution from Sandia will go to support students for lodging and to make up the difference between reduced or waived registration fees for students and actual costs that are incurred for their portion of the meeting space, proceedings, and non-alcoholic meals. Every year about 30% of our attendees are students.

Title: The Linux Cluster Institute's Fifth International Conference on Linux Clusters

PI: Ron Brightwell and Neil Pundit

Dates: May 17-20, 2004

CSRI POC: Neil Pundit, (505) 845-7601

Project Summary:

The Linux Cluster Institute's Fifth International Conference on Linux Clusters will be at the Texas Advanced Computing Center, in Austin, Texas, May 17-20, 2004. This year the Conference will be returning to a format that focuses on the technical, research, and market trends that are shaping the future of Linux HPC. A primary goal of the Conference is to bring vendors, developers, researchers, and users together to share information and plan the future.

Sandia National Lab's prominent role as a sponsor of our past conferences is very much appreciated. This year, with the return to a smaller, more focused venue, the sponsorship opportunities resemble those of prior years. Attached is the Sponsorship package for your perusal. Of course, I'm hoping that SNL will agree again to be a sponsor for the Conference!

Title: Proposal for CSRI Second Sandia Workshop on PDE-Constrained Optimization
"Toward Real-time and Online PDE-constrained Optimization"

PI: Larry Biegler, Carnegie Mellon University
Omar Ghattas, Carnegie Mellon University
Matthias Heinkenschloss, Rice University
David Keyes, Columbia University
Bart van Bloemen Waanders, Sandia National Laboratories

Dates: May 19-21, 2004

CSRI POC: Bart van Bloemen Waanders, (505) 284-6746

Project Summary:

Many engineering and scientific problems in design, control, and parameter estimation can be formulated as optimization problems that are governed by PDEs. The size and complexity of the PDE simulations often present significant optimization challenges. Recent years have seen sustained progress in PDE solvers and optimization algorithms, and the rapid rise in computing capability. Accompanying these advances is a growing interest in real-time and online simulation-based optimization in such diverse areas as aerodynamics, atmospheric and geosciences, chemical process industry, environment, homeland security, infrastructure, manufacturing, and medicine. The need for real-time and online optimization arises in the form of:

- Inverse problems, in which sensor data is repeatedly assimilated into simulations of dynamic processes
- Control problems, in which optimal strategies are repeatedly generated based on new data
- Design problems, in which an optimum is generated rapidly to enable interactive design

The challenges for real-time and online optimization methods include the ability to:
- Run sufficiently quickly for decision-making at relevant time scales
- Adjust to different solution accuracy requirements
- Target time-dependent objectives and constraints
- Tolerate incomplete, uncertain, or errant data

- Be capable of bootstrapping current solutions
- Yield meaningful results when terminated prematurely
- Be robust in the face of ill-posedness
- Scale to large problem sizes and numbers of processors

To discuss research issues associated with overcoming these challenges, the Computer Science Research Institute (CSRI) at Sandia National Labs will sponsor an invitation-only workshop on May 19-21, 2004. This is the second workshop in a series on PDE-based optimization; the first was held in April 2001 (see http://www-2.cs.cmu.edu/~oghattas/pdeopt).

The invited speakers will address the following issues:
- Reduced order modeling within the context of design and control
- Frameworks for real-time and online assimilation and control
- Fast solution methods for time-dependent optimality systems
- Stability, convergence, and regularization issues in the online context
- Applications to problems in aerospace sciences, chemical processes, earth and atmospheric sciences, and medicine

The number of invited speakers has been kept intentionally small, to allow plenty of time for discussion and debate, both formal and informal. In addition to CSRI sponsorship, we anticipate additional support from the National Science Foundation to enable the attendance of graduate students and postdocs. We anticipate publication of a volume on real-time and online optimization in SIAM's Computational Science and Engineering book series (http://www.siam.org/books/compsci.htm), to which workshop participants are invited to contribute a relevant chapter. A volume that came out of the first workshop has been published by Springer: http://www.springer.de/cgi-bin/search_book.pl?isbn=3-540-05045-0.

Title: Proposal for CSRI Workshop on Numerical Aspects of Circuit and Device Modeling (NACDM)

PI: Eric Keiter, Sandia National Labs
Robert Hoekstra, Sandia National Labs
Tom Russo, Sandia National Labs
Jaijeet Roychowdhury, University of Minnesota

Dates: June 23-25, 2004

CSRI POC: Eric Keiter, (505) 284-6088

Project Summary:

Executive Summary: We propose to hold a 3-day workshop with the goal of fostering collaborations between Sandia and the electrical simulation community. Two years ago, in April 2002, a similar workshop was very successful, and opened communication with world experts on numerical analysis, circuit, and device simulation. Much of this communication has lead to development of several new, innovative algorithms for the ASCI Xyce™ Parallel Electronic Simulator.

Having a follow-up workshop will allow us to extend those relationships and also provide a forum for new topics and ideas to be discussed. The Xyce™ simulator not only needs to support scalable solution of very large problems (>million devices), but a broad range of physics and fidelity are also necessary, ranging from semiconductor device simulation to mixed signal analysis.

Topics: The topics that we are concerned with include:
• Stiff, coupled time-dependent ODE/DAEs.
• Large-scale nonlinear systems
• Ill-conditioned, indefinite sparse linear systems.
• Partitioning and load balance.
• Constrained optimization and sensitivity analysis.
• Semiconductor device simulation.
• Algorithms for mixed-signal analysis, and other multi-fidelity algorithms.

Goals: The specific goals of the workshop are to:
- Foster and strengthen collaborations between Sandia and leaders in electrical simulation and numerical analysis.
- Exchange information on the state-of-the-art methods for linear systems, nonlinear equations, ODE/DAEs and PDEs as applied to circuit and device simulation.
- Assess algorithmic requirements and challenges for continued advancement of scalable parallel solution of electrical circuit and device problems.

Format: We propose that the workshop will be held April 21-23, 2004, at The Eldorado Hotel in Santa Fe, NM. Each day will consist of two presentation sessions and one discussion session. The presentation sessions will consist of 3-4 30-minute presentations. The discussion session will be 1-2 hours and consist of break-out groups focused on specific discussion topics which summaries from each break-out group at the end of the session. Approximately half of the sessions will focus on the numerical aspects of circuit simulation (linear systems, nonlinear equations, time integration of ODE/DAEs). The remaining half will focus on electrical simulation of different fidelity, such as device simulation (PDE) and mixed-signal simulation. The presentations will be collected and posted online after the workshop.

Title: Proposal for CSRI Workshop on Multiscale Mathematics

PI: Richard Lehoucq, Sandia National Laboratories
Scott Collis, Sandia National Laboratories

Dates: December 13-15, 2004

CSRI POC: Richard Lehoucq, (505) 845-8929

Project Summary:

Motivation:
The DOE office of science has conducted three workshops on multiscale mathematics during the past calendar year in preparation of an RFP in multiscale mathematics. The broad consensus of the works is that simulation over a broad range of scales in needed for tomorrow's science based efforts in science and engineering. The following are three questions for driving the proposed workshop.

1. What the appropriate driving applications/ideas for a response to the RFP? Given that available funding for the entire RFP is likely to be 8-9 million dollars, how should Sandia structure our response to the RFP? Specifically, by structure we mean partnerships with university faculty and other labs, the number and size of the proposals. Ideally, our proposals should separate Sandia from the other labs and emphasize our strengths. Therefore, what are Sandia's strengths that are synergistic with multiscale mathematics and science?
2. What are the multiscale aspects of the possible projects that are candidates for proposals? For example, does the problem exhibit a solution(s) that possesses multiscale characteristics (for instance turbulence) or couple disparate regimes (continuum to MD)? Along these lines, does the project push a multiscale math or science objective?
3. What is an example simulation that contains sufficient multiscale to exploit Sandia's strengths in large-scale simulations driven by algorithm analysis? For example, a continuum to MD simulation leverages Sandia's existing strengths.

Purpose of the Workshop
The goal of the workshop is to bring together a small group of scientists to discuss current and potential synergistic efforts in multiscale mathematics and applications. This workshop will allow Sandia to develop a roadmap and foster collaborations in multiscale mathematics and science. We believe this activity will serve as a catalyst to accelerate further developments and ensure that Sandia National Laboratories is a world-class leader in multiscale mathematics and science.

Our preliminary agenda is to alternate between lectures and breakout discussions. The afternoons and mornings can alternate between mathematics and applications, respectively. Everything should be completely Sandia centric and the lectures should focus on research issues, open questions, and potential research directions. The discussions should be (strongly) moderated to keep them on target and Sandia centered.

Chapter 5. Seminar Abstracts

The CSRI hosts an active short-term visitor program, which is closely aligned with a seminar schedule. Short term visit typically last between two days and two weeks and include a seminar as well as a broad range of meetings and collaborations with Sandia staff. The longer visits are encouraged to increase the likelihood that a significant collaboration will develop. The abstracts for the CSRI seminars are listed below in alphabetical order by speaker.

Title: Reliability-Based Analysis and Design Optimization of Aerospace Systems

Speaker: Matthew Allen, University of Colorado at Boulder

Date/Time: August 11, 2004, 10:00-11:00 am (MDST)

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Multiphysics phenomena are often only roughly approximated when the stochastic nature of a system is considered in the design optimization process. This leads to potentially significant epistemic uncertainties while attempting to quantify the effects of system uncertainties. A computational framework is presented that integrates high-fidelity multiphysics models, namely aeroelastic and electrostatic, into reliability-based design optimization (RBDO) processes. The first order reliability method (FORM) is implemented and verified by numerical studies demonstrating that highly nonlinear systems do not necessarily result in nonlinearities in the standard normal uncertainty space. The effects of uncertainties, and the level of uncertainties, on the design process are studied for various wing structures and MEMS devices. Though the coupling of FORM and efficient gradient-based optimization algorithms has allowed for RBDO of steady-state systems, the additional cost of dynamic analysis renders existing frameworks infeasible for real world dynamic systems. Reduced order modeling (ROM) techniques have proven to be a useful tool in reducing computational costs, but are generally only applicable to the specific model for which it was built, which renders the ROM unusable for analyzing an altered system. A ROM is proposed that can be extended into the parametric spaces of design and random variables. With such a ROM, referred to as an extended reduced order model (EROM), the computational costs of analyzing altered designs are minimized, thus enabling a RBDO framework. The accuracy, convergence, and computational cost of the optimization process utilizing the EROM is compared to a traditional optimization process utilizing the full order system each iteration.

CSRI POC: Michael Eldred, (505) 844-6479

Title: Genomic Signal Processing: Large-Scale Data, Matrix (and Tensor) Algebra and Basic Biological Principles

Speaker: Orly Alter, University of Texas, Austin

Date/Time: Thursday, December 9, 2004, 10:00 - 11:00 am (CA)
11:00 - 12:00 pm (NM)

Location: Building 915, Room W133 (Sandia CA)
Building 980, Room 24 (Sandia NM)

Brief Abstract: The sequencing of the human genome and of the genomes of several model organisms is already completed or well underway. Recent advances in high-throughput technologies enable acquisition of different types of molecular biological data, monitoring the flow of biological information as DNA is transcribed to RNA, and RNA is translated to proteins, on a genomic scale. Laboratories all over the world are generating vast quantities of genomic data in studies of cellular processes, regulatory programs and tissue samples. Future predictive power and discovery in biology and medicine will come from the mathematical modeling of these datasets, which hold the key to fundamental understanding of life on the molecular level, as well as answers to questions regarding medical diagnosis, treatment and drug development.

I will describe the first data-driven models for large-scale molecular biological data using tools from matrix algebra, singular value decomposition (SVD), generalized SVD (GSVD) and pseudoinverse projection. The mathematical variables of the SVD and GSVD models, i.e., the "eigengenes" and "eigenarrays" patterns, or the "genelets" and "arraylets" patterns, that they uncover in the data, appear to represent independent processes and corresponding cellular states (such as observed genome-wide effects of known regulators, the biological components of the cellular machinery that generate the genomic signals, and measured samples in which these regulators are over- or underactive) .The mathematical operations of these models, i.e., data reconstruction and classification in the subspaces spanned by these eigengenes and eigenarrays, or genelets and arraylets, appear to simulate experimental observation of the processes and cellular states, respectively, that these patterns represent. I will illustrate these models in analyses of time course and tumor sample data.

Finally, I will illustrate the ability of these models to uncover basic cellular biological principles (3): Mapping genome-scale protein binding data using pseudoinverse projection onto patterns of RNA expression data that had been extracted by SVD and GSVD, a novel correlation between DNA replication initiation and RNA transcription during the cell cycle in yeast is predicted.

(1) Alter, Brown & Botstein, PNAS 2000; www-genome.stanford.edu/SVD
(2) Alter, Brown & Botstein, PNAS 2003; www-genome.stanford.edu/GSVD
(3) Alter & Golub, to be published in PNAS; www.med.miami.edu/mnbws/Alter-.pdf

CSRI POC: Genetha Gray, (505) 294-4957

Title: Energy Stable Discretization of Compressible MHD: Theory and Implementation

Speaker: Tim Barth, NASA Ames Research Center

Date/Time: Monday, August 16, 2004, 1:30-2:30 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: A self-contained energy analysis is briefly outlined for the discontinuous Galerkin (DG) discretization (Reed and Hill [1]) applied to the compressible magnetohydrodynamic (MHD) equations with solenoidally constrained magnetic induction field, div(B)=0. This analysis quantitatively reveals why discretization of the MHD equations is fundamentally more demanding than either the Maxwell or hydrodynamic equations alone. Unlike standard hydrodynamics (see for example Barth [2]), the DG energy analysis for MHD reveals the subtle role of the solenoidal constraint in obtaining global and elementwise local stability through

- strong or weak satisfaction of div(B)=0 in element interiors
- strong or weak satisfaction of B*n=0 on element interfaces.

The theory suggests several discontinuous Galerkin discretization strategies for compressible MHD depending on whether each condition is strongly or weakly enforced. Some strategies are quite simple in theory but can be overly complicated in practical implementation.

In the remainder of the lecture, we discuss these various strategies with emphasis given to implementation issues and quality of numerical results when applied to demanding MHD problems.

[1] Reed and Hill, 'Triangular Mesh Methods for the Neutron Transport Equation", LANL Report UR-73-479, 1973.

[2] Barth, "Simplified Discontinuous Galerkin Methods for Systems of Conservation Laws with Convex Extension", Springer, LNCSE, Vol. 11,
1999.

CSRI POC: Mark Christon, (505) 844-8279

Title: Projection Methods for Reduced Order Modeling

Speaker: Christopher Beattie, Virginia Polytechnic Institute and State University

Date/Time: Monday, March 15, 2004, 1:00 - 2:00 pm

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: Direct numerical simulation has been one of few available means for the systematic study of physical phenomena for which experiments are dangerous, expensive, or illegal to perform. But the burdens of complex geometries, multiphysics, and hostile operating environments coupled with the ever increasing need for accuracy and model fidelity make scalable simulation at best unlikely without some systematic strategies for reducing model complexity.

This talk describes a variety of projection methods for model reduction that seek to replace large-scale or infinite-order dynamical systems arising from PDE models with a system of relatively low dimension that ideally will have the same response characteristics as the original system, yet require far less computational intensity for realization than the intractable levels the original system may have required. The methods originate in the same family as POD/Kahunen-Loeve methods (which will be introduced as well) yet they take into greater account the features of the original PDEs, discretization strategies, and solution functionals of interest. We discuss various weighting paradigms in POD, connections with Krylov decompositions, and their analogs in the original PDE setting.

CSRI POC: Rich Lehoucq, (505) 845-8929

Title: A parallel multilevel preconditioner for the p-version of the Finite Element Method

Speaker: Sven Beuchler, Johan Radon Institute for Computational and Mathematics

Date/Time: Monday, March 1, 2004, 10:00-11:00am (PST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: In this talk, a uniformly elliptic second order boundary value problem in 2D is discretized by the p-version of the finite element method. An inexact parallel Dirichlet-Dirichlet domain decomposition pre-conditioner for the system of linear algebraic equations is investigated. Using methods of multi-resolution analysis, we propose optimal preconditioners for Schur complement, the solver on the subdomains and the extension operating from the edges of the elements into their interior. On the one hand, a suboptimal condition number estimates are given, on the other hand numerical experiments on the parallel computer show the performance and speed up of the proposed methods.

CSRI POC: Jonathan Hu, (925) 294-2931

Title: Mondriaan sparse matrix partitioning

Speaker: Rob Bisseling , Utrecht University

Date/Time: Thursday, May 13, 2004, 3:00-4:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Mondriaan is a two-dimensional, multilevel, hypergraph-based package for the partitioning of a rectangular sparse matrix, to be used as a sequential preprocessing step for parallel sparse matrix-vector multiplication. In this talk, the Mondriaan approach will be explained and its performance will be compared with geometric partitioning for finding the minimum-energy configuration of a 20,000-particle sample of amorphous silicon. The geometric partitioning is based on BCC sphere packing. Furthermore, we show how the communication load of the multiplication can be balanced among the processors.

CSRI POC: Karen Devine, (505) 845-7585

Title: Highly Scalable Data Intensive Computing and Genomic Sequence Analysis--A New Architectural Approach

Speaker: Bill Blake, SVP Product Development, Netezza Corporation
Barry Zane, VP Technology

Date/Time: Friday, May 14, 2004, 11:00-12:00 noon

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Today, organizations need to analyze billions of records in increasingly short time periods to support business decisions--an area known as Business Intelligence. Netezza has developed a merged server/parallel relational database/storage product that can process very complex ad hoc queries on extremely large data sets with response times 50X to 100X that typically delivered by large scale SMP or cluster of SMP systems.

This presentation will describe the Asymmetric Massively Parallel Processing architecture of the Netezza Performance Server. Of particular note is the coupling of a front-end Linux SMP node for parallel query compilation and optimized execution planning with a highly parallel back end of computing nodes that employ a light-weight kernel and specialized datapath logic for processing records as they stream off the disk. Overall, the Netezza approach is an interesting example of the co-design of hardware and software of an application focused complex system—a scalable analytic database in this case. In addition, extensions of the SQL capability to include genomic sequence analysis within the parallel relational engine will be discussed.

Part of the intent of this presentation is to prompt discussion on ways data intensive computing can be coupled with "classic" massively parallel high performance computing.

CSRI POC: Lee Ward, (505) 844-9545

Title: Solving Optimization Problems for Protein Structure Prediction

Speaker: Richard Byrd , University of Colorado at Boulder

Date/Time: Tuesday, March 2, 2004, 10:00-11:00 am (PST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: In this talk we discuss effective optimization algorithms for prediction for prediction of protein structure by energy minimization. The protein structure prediction problem is to predict the three-dimensional shape, or native state of a protein, given its sequence of amino-acids. Optimization is one of the promising approaches to solving this problem, because it is believed that in most cases, the native state corresponds to the minimum free energy of the protein.

However, the energy landscape of a realistic-sized protein has thousands of parameters and an enormous number of local minimizers.

We have developed a large-scale global optimization algorithm for solving this problem. Results from the CASP competition show our method to be particularly successful on protein targets where structural information from similar proteins is unavailable. The method makes use of random sampling, secondary structure predictions, subspace minimization, and a lot of unconstrained local optimization. In this talk we focus on a preconditioned limited memory quasi-Newton method we have recently developed. We use automatic differentiation to compute the second derivative of the bonded terms in the energy, which form a banded Hessian. So far this approach has resulted in significant speed-ups in solution time.

CSRI POC: Paul Boggs, (925) 294-4630

Title: Progress and Challenges in Modeling and Unstructured Grid Computations

Speaker: Professor Graham F. Carey, The University of Texas at Austin

Date/Time: Thursday, August 12, 2004, 11:00-12:00 noon

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: The challenge of mesh generation and enhancement is introduced here in the broader context of the end-to-end analysis, visualization and optimal design problem. In particular, it impacts some aspects of geometric design and shape treatment as well as the analysis and design engineering problem. Modeling error and optimal control for a targeted result are considered here in relation to the role of meshing and the need to treat both multi-scale and multi-physics. Adaptive strategies clearly play an important role in addressing these problems and some of our recent work with adaptive mesh refinement algorithms, error indicators and software libraries will be summarized and illustrated by application studies. Some related work on constrained mesh enhancement and other ongoing mesh studies will be presented as time permits

CSRI POC: Patrick Knupp, (505) 284-4565

Title: History in Hysteresis: Critical Scaling in Noisy, Disordered Systems

Speaker: John H. Carpenter, University of Illinois, Urbana-Champagne

Date/Time: Tuesday, July 13, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: The effect of history on avalanche type behavior in driven, disordered systems, such as Barkhausen noise in magnets, is studied using the non-equilibrium, zero temperature random-field Ising model. A numerical scaling analysis of avalanche size distributions, correlation functions, and spanning avalanches for the AC demagnetization curve reveals a phase transition as the disorder is tuned, similar to that of the saturation hysteresis loop. Furthermore, a scaling analysis for nested, concentric, symmetric subloops performed via the introduction of a history-induced disorder parameter also shows critical behavior. The critical exponents for both cases are related and found to be consistent with the saturation loop exponents plus one possibly new exponent. Next, the effects of long range demagnetizing fields are shown to produce self-organized critical type behavior in both the demagnetization curve and subloops. Finally, subloop measurements for thin film magnets and a soft ferromagnet produce good qualitative agreement with the model.

CSRI POC: John Aidun, 9235, (505) 844-1209
Chris Deeney, 1646, (505) 845-3657

Title: Interfacial Equilibria and Structure of Polyatomic Fluids from Interfacial-SAFT (*i*SAFT) Density Functional Theory

Speaker: Walter Chapman and Sandeep Tripathi, Rice University

Date/Time: Wednesday, September 29, 2004, 10:00-11:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: A wide range of potential applications such as environmental remediation, biochemical separations, design of biosensors, catalysis, wettability etc. have created significant interests in molecular level studies of systems of complex fluids (e.g. hydrogen bonding fluids, hydrocarbons, proteins, polymers) at solid-fluid and fluid-fluid interfaces. Experimental studies of such systems are challenging due to the small scale of the system. Although computer simulations do help overcome some of these problems, they are computationally expensive; hence the importance of accurate theories cannot be overemphasized.

We have developed a density functional theory (DFT) based on Wertheim's theory of associating fluids that is capable of modeling the adsorption, phase and even chemical equilibria of mixtures of associating and reacting polyatomic fluids near hydrophobic and hydrophilic surfaces. The density functional theory is based on the same formalism as the SAFT model that is widely applied to model bulk phase behavior of associating fluids and polymer solutions. Comparing with Monte Carlo simulations, we demonstrate the success of the DFT in capturing the effects of size and shape of the fluid molecules, system parameters such as fluid-fluid and surface-fluid association/interaction strengths and hydrophobicity of the surface, on fluid structure and interfacial properties.

CSRI POC: Laura Frink, (505) 844-1910

Title: Convergence Examples of a Filter-Based Evolutionary Algorithm

Speaker: Lauren Clevenger, University of New Mexico

Date/Time: Wednesday, June 16, 2004, 10:00-11:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: We describe and critique the convergence properties of filter-based evolutionary pattern search algorithms (F-EPSAs). F-EPSAs implicitly use a filter to perform a multi-objective search for constrained problems such that convergence can be guaranteed. We provide two examples that illustrate how F-EPSAs may generate limit points other than constrained stationary points. F-EPSAs are evolutionary pattern search methods that employ a finite set of search directions, and our examples illustrate how the choice of search directions impacts an F-EPSA's search dynamics.

Lauren is a student intern in 9215, who has been working with Bill Hart on the analysis of pattern search methods this past year. Lauren's presentation is a dry run for her talk at the upcoming GECCO conference.

CSRI POC: Bill Hart, (505) 844-2217

Title: DACHE: Direct Access Cache System for I/O

Speaker: Kenin Coloma, Northwestern University

Date/Time: Wednesday, September 8, 2004, 2:00pm (MDST)

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: DACHE is a client-side file caching library with its notable characteristics being coherence, scalability, and a passive architecture. DACHE keeps up to one copy of any given cache page across the entire system. Any page cached can be accessed by any other process using Remote Memory Access. The single-cached-copy design ensures cache coherence. By distributing much of the book keeping and management, DACHE sidesteps potential bottlenecks. The passive nature of DACHE is born out of both necessity and efficiency. Sandia has adopted a threadless approach to compute nodes, ruling out the active coordination of processes with threads. RMA allows for both data transfer and the passive manipulation of distributed state, minimizing interference with remote processes.

CSRI POC: Sonja Tideman, (505) 284-0268

Title: Performance Analysis of Trilinos Mathematical Solvers on Next-Generation Processors

Speaker: Professor Jeanine Cook, New Mexico State University

Date/Time: Thursday, April 29, 2004, 10:00-11:00 am

Location: Building 980 Room 24 (Sandia NM)

Brief Abstract: As performance improvements between successive processor generations begin to level off, it becomes increasingly important to understand the behavior of applications on the underlying processor microarchitecture to determine the best match between application and processor for performance optimization. Through studying trends and the projected improvements in semiconductor technology, we can predict the size and structure of future commodity processors. In this talk, we present the methodology and techniques that we are currently using to analyze the performance and characterize the behavior of Trilinos, a large collection of mathematical solvers, on current and future microarchitectures. An outline of the project and preliminary results will be presented.

CSRI POC: Erik P. DeBenedictis, (505) 284-4017

Title: Multidisciplinary Analysis and Optimization

Speaker: Professor Brian H. Dennis, The University of Tokyo

Date/Time: Thursday, April 15, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: This lecture will conceptually summarize and briefly animate my diverse work in multidisciplinary forward and inverse analysis and design optimization. The results to be presented will involve:

Multidisciplinary Analysis
- A 2-D *h/p*-version least-squares finite element method (LSFEM) for electromagnetohydrodynamics
- Magnetohydrodynamic suppression of thermally driven flow in silicon crystal growth
- Magnetohydrodynamic control of diffuser flow
- Suppression of cylinder wake vortices with an electromagnetic field
- Simulation of cooling of a realistic 3-D human head and brain

Design Optimization
- Shape optimization of turbine blade coolant passages with parallel FEM analysis
- Multi-objective constrained shape optimization of a turbine cascade
- Aerodynamic shape optimization of a transonic wing using globally distributed computing resources

Inverse Problems
- A finite element method for inverse detection of boundary conditions in 2-D and 3-D thermoelasticity

CSRI POC: Pavel Bochev, (505) 844-1990

Title: A Fast Multigrid Method for Inverting Parabolic Problems

Speaker: Andrei Draganescu, University of Chicago

Date/Time: Monday, May 10, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)
Building 912 Room 180D (Sandia CA)--videoconference

Brief Abstract: This work started as a bid for a cost-efficient method for inverting time-dependent partial differential equations. The original motivation comes from the problem of comparing simulations with experimental results in order to improve the knowledge about the initial conditions and problem parameters. Since this problem is in general ill-posed, we treat it as a regularized optimization problem, controlled by a possibly large set of parameters that includes the whole initial state. The goal is to solve the inverse problem at a cost no larger than, say, ten forward problems, a demand that is challenged by the large size of the control-space. We propose a multigrid-like algorithm that fulfills this requirement in case the forward problem is of parabolic type. The methods we propose can potentially be extended to inverse problems for fluid flow.

CSRI POC: Bart van Bloemen Waanders, (505) 284-6746

Title: Multi-Objective Design Optimization: Formulation, Solution and Implementation

Speaker: John Eddy, Ph.D., Interview Candidate , University at Buffalo, State University of New York (SUNY)

Date/Time: Tuesday, July 20, 2004, 9:00-10:00 am (PDT)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: Consideration for more than one competing measure of performance or objective is often necessary in the design of engineering artifacts. Optimization problems formulated with regard to each such objective are called multi-objective optimization problems. Such problems differ from single objective problems in that the objective function is vector valued as opposed to scalar valued. While the solution to a single objective optimization problem is typically a single point representing the best possible design configuration, the solution to an interesting multi-objective optimization problem is a potentially infinite set of design configurations known as the Pareto optimal set. Finding this set of solutions is one of the biggest challenges in a multi-objective design problem. In this talk, I will discuss common methods of solving multi-objective problems and the advantages and pitfalls of such approaches. I will then discuss the use of evolutionary algorithms to seek the entire Pareto optimal set of solutions in a single optimization phase along with the advantages and pitfalls of that approach. I will demonstrate the ability of evolutionary algorithms to provide the desired solution sets for some small scale optimization test problems and discuss current work involving large scale, high-fidelity, high dimensional industrial optimization problems. I will also discuss work implementing multi-objective optimization concepts in multi-agent systems to solve decentralized, non-cooperative design problems. The challenge of this work is to find an equivalently effective solution to the decentralized problem with incomplete information as can be found in a centralized problem with complete information.

CSRI POC: Laura Painton Swiler, (505) 844-8093

Title: Fourier Analysis of Multigrid for the Two-Dimensional Convection-Diffusion Equation

Speaker: Howard Elman, University of Maryland
Alison Ramage, University of Strathclyde

Date/Time: Tuesday, June 8, 2004, 10:00-11:00 am (PDST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: We present an analysis of multigrid methods for a constant-coefficient model convection-diffusion equation discretized using bilinear elements. We show that this model problem on an n x n grid can be transformed using Fourier methods to a set of n independent problems that have the tridiagonal structure of one-dimensional problems, and that to a great extent this one-dimensional structure is preserved when a multigrid solver is applied. This structure is then used to explore the behavior of multigrid. In particular, it is shown that the behavior of multigrid for Dirichlet problems can be predicted by its behavior for certain related periodic problems.

CSRI POC: Vickie Howle, (925) 294-2204

Title: Generalized Green's Functions and the Effective Domain of Influence

Speaker: Donald Estep, Colorado State University

Date/Time: Thursday, February 5, 2004, 2:00-3:00 pm (MST)

Location: Building 980 Room 95 Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: One well-known approach to a posteriori analysis of finite element solutions of elliptic problems estimates the error in a quantity of interest in terms of residuals and a generalized Green's function. The generalized Green's function solves the adjoint problem with data related to a quantity of interest and measures the effects of stability, including any decay of influence characteristic of elliptic problems. We show that consideration of the generalized Green's function can be used to improve the efficiency of the solution process when the goal is to compute multiple quantities of interest and/or to compute quantities of interest that involve globally-supported information such as average values and norms. In the latter case, we introduce a solution decomposition in which we solve a set of problems involving localized information, and then recover the desired information by combining the local solutions. By treating each computation of a quantity of interest independently, the maximum number of elements required to achieve the desired accuracy can be decreased significantly.

CSRI POC: David Ropp, (505) 845-7431

Title: A Model for Dynamic Load Balancing on Heterogeneous and Non-Dedicated Clusters

Speaker: Jamal Faik, Rensselaer Polytechnic Institute

Date/Time: Tuesday, January 20, 2004, 7:00-8:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: As clusters become increasingly popular alternatives to custom-built parallel computers, they expose a growing heterogeneity in processing and communication capabilities. Performing an effective load balancing on such environments can be best achieved when the heterogeneity factor is quantified and appropriately fed into the load balancing routines. In this work, we discuss an approach based on constructing a tree model that encapsulates the topology and the capabilities of the cluster. The different components of the execution environment are dynamically monitored and their processing, memory and communication capabilities are collected and aggregated in a simple form easily usable when load balancing is invoked. We used the model to guide load balancing in the solution of a two-dimensional Rayleigh-Taylor instability problem on a heterogeneous Sun cluster. We have observed a decrease of up to 18% in execution time out of a theoretical maximum of 20%.

CSRI POC: Karen Devine, (505) 845-7585

Title: Multiscale Computational Framework for Transient Problems

Speaker: Jacob Fish, Rensselaer Polytechnic Institute

Date/Time: Tuesday, May 25, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: In this talk I will discuss various multiscale computational approaches for transient problems aimed at predicting dynamic response of engineered components and structures including complex failure mechanisms operating at multiple temporal and spatial scales. The dynamic behavior of structural systems is assessed from the fundamental physical processes operating at smaller spatial and temporal scales than currently resolved in simulations.

The focus of this talk will be on modeling of fatigue and impact - two problems that exhibit multiple temporal scales. Using recently developed temporal homogenization theory for non-periodic fields the initial-boundary value problem corresponding to fatigue is decomposed into: (i) the macro-chronological initial-boundary value problem with smooth loading for the entire loading history, and (ii) the micro-chronological initial-boundary value problem with the oscillatory portion of loading for a single load period in selected region(s) of the time domain. Large time increments are used for the macro-chronological problem, while the integration of the micro-chronological initial-boundary value problem requires a significantly smaller time step. This approach allows for a rigorous modeling of fatigue and life time predictions, which are not based on S-N curves or Goodman-type diagrams.

Recent experiments conducted on impact of composite tubes [1] showed a clear tendency toward lower strain energy absorption at higher crush rates - a surprising phenomenon that cannot be explained by current modeling and simulation practices. Due to coupling between spatial and temporal scales, dynamic properties of heterogeneous materials have been shown to significantly differ from those obtained in quasistatic loading conditions. Quasistatic design methods are too restrictive since they do not take into account the ability of materials to disperse energy and momentum from the applied transient loading. The small-scale heterogeneity could lead to scattering of waves, which may be reflected in the rise time of shock waves.

[1] M.E. Botkin, “Crash Prediction of Composite Structures” private communications, May, 2003.

CSRI POC: John Aidun, (505) 844-1209

Title: Progress on discrete-to-continuum bridging methodologies

Speaker: Jacob Fish, Rensselaer Polytechnic Institute

Date/Time: Tuesday, June 1, 2004

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: In this talk, I will present information-passing and concurrent discrete-to-continuum bridging methodologies. In the concurrent approach both, the discrete and continuum scales are simultaneously resolved, whereas in the information-passing schemes, the discrete scale is modeled and its gross response is infused into the continuum scale. Among the information-passing bridging techniques, I will present the generalized mathematical homogenization method, the model reduction method as well as the generalization of the Partition of Unity Method (PUM) to discrete scales. The extended PUM method gives rise to the enriched quasi-continuum formulation, capable of dealing with heterogeneous inter-atomic potentials as well as with high velocity impact problems. Among the concurrent bridging techniques, attention is restricted to multigrid (multilevel) methods.

CSRI POC: John Aidun, (505) 844-1209

Title: Algebraic Modeling Language Support for Combinatorial Optimization

Speaker: Robert Fourer, Northwestern University

Date/Time: Monday, December 13, 2004, 10:00-11:00 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: Algebraic modeling languages are widely used in formulating and solving broad classes of optimization problems, particularly linear, quadratic, and smooth nonlinear programs. But they have proved much less helpful for working with combinatorial optimization problems, for which their applicability has largely been limited to reformulations as integer programs. For important classes of combinatorial problems such as scheduling, sequencing, routing, and assignment, equivalent integer programs do not provide the sort of natural problem description that is the major motivation for modeling languages. Solvers designed for integer programming also often fail to work well on these formulations.

A variety of extensions to algebraic modeling language syntax -- including logical, conditional and counting operators, variables in subscripts, and object-valued and set-valued variables -- can make such languages much more natural and useful. Nevertheless, for many years extensions like these were of limited interest, because there were no readily available general-purpose solvers to deal with problems expressed in these ways. This situation began to change only with the advent of sophisticated constraint programming solvers that could directly address the natural formulations of many combinatorial problems. In reaction to the success of constraint programming, moreover, there has also come a better appreciation of how combinatorial modeling language expressions can be automatically converted to strong integer programming formulations.

This survey will present a variety of examples, taken mainly from ongoing extensions to the AMPL modeling language and a corresponding driver for ILOG's Optimization Suite using their Concert Technology interface.

CSRI POC: David M. Gay, (505) 284-1456

Title: Reversible Supercomputing, Beyond the Limits of Moore 's Law

Speaker: Michael Frank, University of Florida

Date/Time: Wednesday, May 12, 2004, 2:00-3:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Moore's Law will hit a fundamental brick wall in roughly 20 years (if not sooner), as device sizes approach the nanometer scale, and bit energies concurrently approach a lower bound of ~100 kT required for reliability. As one consequence, a 100W processing node with 10^8 gates (as exist today) could never run faster than ~2.4 THz if these bit energies are to be entirely dissipated on each cycle into a room-temperature environment. Note that this represents only about 10 doublings (or 15-20 Moore's Law years) in power-performance beyond present-day processors.

Moreover, not only standard CMOS, but also *any possible* nanocomputing technology that remains based on the traditional "irreversible" computing paradigm suffers from this same sort of constraint on power-performance. Irreversible logic, by definition, relies on continual erasure of old logic outputs, overwriting them with new ones. The energy dissipated per bit-erasure can be reduced to no less than ~.7kT, even in the best case of a degenerate nano-device in which the erasure is carried out via an isothermal compression of the phase space.

Clearly, in order for there to be any hope of continuing power-performance improvements beyond the near future, we need to seriously consider what is, by definition, the only possible alternative to irreversible computing: reversible computing. In reversible computing, we *decompute* unwanted bits, rather than erasing them, which allows us to carry out bit transitions adiabatically via ballistic processes, with losses potentially <<kT. Reversible computing imposes some overhead in terms of logic hardware complexity, but it *improves* overall system cost-efficiency whenever the cost of energy, and/or cooling constraints, are dominant limiting factors on performance. Moreover, cooling becomes an increasingly stringent limiter of moderately tightly-coupled parallel 3D-mesh computations, as the problem size increases.

Contrary to some widespread myths, reversible computing violates no laws of physics, nor does it render computer design inordinately more difficult. Conversion of traditional logic designs to mostly-reversible ones can be mostly automated, although hand-optimization can still achieve even higher efficiency in many cases. Reversible computing does require high-Q ballistic devices to carry out most energy transfers, and in the SRC-funded reversible computing project at UF, we are presently designing custom RF MEMS resonators to serve this role in near-term reversible CMOS processors.

This presentation is relevant to the future of high performance supercomputing and very low power computing. Some prototype implementations use RF MEMs resonators as a key part of the power system.

CSRI POC: Erik DeBenedictis, (505) 284-4017

Title: A Combined Mechanical/Multilevel Preconditioning in Nonlinear Shell Mechanics

Speaker: Michael Gee, University of Stuttgart, Germany

Date/Time: Monday, March 8, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: The analysis of large-scale nonlinear shell problems asks for parallel simulation approaches. One crucial part of efficient and well scalable parallel FE-simulations is the solver for the system of equations. Due to the inherent suitability for parallelization one is very much directed towards preconditioned iterative solvers. However thin walled structures discretized by finite elements lead to ill-conditioned system matrices and therefore performance of iterative solvers is generally poor. This situation further deteriorates when the thickness change of the shell is taken into account. A preconditioner for this challenging class of problems is presented combining two approaches in a parallel framework. The first one is based on a scaling of the shell director. The second approach utilizes an aggregation multigrid concept.

It is demonstrated by several numerical examples that both approaches allow to remedy the ill-conditioning of the underlying problem.

CSRI POC: Jonathan Hu, (925) 294-2931

Title: A hierarchical modeling approach to disparate time simulation: connecting metabolic rate and temperature to population growth rates in marine

Speaker: Damian Gessler, National Center for Genome Resources (NCGR)

Date/Time: Wednesday, January 28, 2004, 9:30-10:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: We present a computational and a scientific model that connects sub-cellular with macro-ecological processes. The computational model uses an event-driven paradigm in an hierarchical framework to connect disparate-time processes in a single simulation. The connection across hierarchical levels is done via a loose-coupling of suppliers and listeners to parameterized values; the connection across temporal scales is achieved by synchronizing event clocks to a shared master clock, whereby the master clock orchestrates event delivery so that all events are delivered in monotonically increasing temporal order.

The scientific model is based on the last half-decade of work connecting body mass and temperature to metabolic rate, and metabolic rate to population parameters such as growth rates and energy flux. This work has developed broad-sweeping models for macro-ecology, offering macro-scale explanations based on micro-scale mechanisms. As such, it is a powerful model to connect hierarchical levels. One of the predictions of the model is the Energy Equivalence Rule, which predicts a conserved energy flux across trophic levels. We present the first implementation of this scientific model in the framework of the hierarchical computational model.

Authors: Damian Gessler, Andrea Belgrano, and Peter Steadman, (NCGR)

CSRI POC: Danny Rintoul, (505) 844-9592

Title: Superfast Nested Dissection

Speaker: Ming Gu, University of California, Berkeley

Date/Time: Tuesday, April 13, 2004, 4:00-5:00 pm

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: We develop stable and nearly linear time direct solvers for linear equations arising from finite difference/finite element discretization of large classes of 2D partial differential equations. It has been known for three decades that the nested dissection method (ND), which takes O(n^3) time to solve these equations on an n-by-n square grid, has the optimal complexity. Yet, our method would only require O(n^2 p) time, with p a modest parameter dependent on a user-prespecified tolerance. This work can be generalized to arbitrary regions and to 3D for a large number of PDEs.

CSRI POC: Rich Lehoucq, (505) 845-8919

Title: Approximation and Control of Large-Scale Dynamical Systems via Krylov Projection Methods

Speaker: Serkan Gugercin, Virginia Polytechnic Institute and State University

Date/Time: Monday, March 15, 2004, 2:00-3:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Simulations in large-scale settings often lead to unmanageably large demands on computational resources and provide, as a consequence, the main motivation towards the development of effective methods for model reduction. The resulting low order (yet high fidelity) model can be used to replace the original system as a component in a larger simulation or it might be used to develop a fast and simple reduced order controller suitable for real time applications.

In this talk, we introduce computationally efficient methods to construct reduced order models via Krylov projections for both simulation and control of large-scale dynamical systems. By applying Krylov projection techniques to optimize certain performance measures, these new tools yield satisfactory model approximations within guaranteed performance margins in a numerically efficient and stable manner.

For simulation-based model reduction, we propose a strategy for choosing optimal interpolation points (shifts) for Krylov projection. For control-based model reduction, we are able to produce in a numerically efficient manner a reduced order controller via Krylov projection, which both approximates the full order controller, and further, creates the same closed loop behavior as the original controller. Several numerical examples will be presented to illustrate the effectiveness of the proposed approaches.

CSRI POC: Rich Lehoucq, (505) 845-8929

Title: Photonically-Enabled CMOS

Speaker: Cary Gunn, Luxtera Inc.

Date/Time: Wednesday, December 09, 2004, 3:00-4:00 p.m.

Location: Building 980, Room 24 (Sandia NM)

Brief Abstract: Over the past 3 years Luxtera has developed advanced photonic capability within the confines of a commercially available 0.13um CMOS process. Using nearly identical design rules as those allowed in the basic CMOS design, Luxtera is able to implement optical waveguiding, filtering, modulation, switching, and detection at speeds of 10Gb/s and above. This has been achieved by applying a unique simulation capability to the design of silicon nanophotonic components, and by a rigorous adherence to the process requirements of CMOS transistors. As a result, Luxtera is able to design a completely integrated chip that both digitally processes data using CMOS transistors and optically transports data using integrated optical components.

Luxtera's technology is being developed to support a broad array of defense and commercial applications including low cost DWDM digital and analog data links, optical beam steering, resonant optical gyroscopes, and low phase noise RF oscillators. DARPA has recently selected Luxtera for a $12M contract to develop a small form factor single chip transceiver that uses on-chip DWDM to multiplex ten 10Gb/s channels onto a single fiber.

In this talk, Luxtera will discuss the techniques that have been used to develop the technology, and some characteristics of the resulting library of components that may be used to build CMOS electro-optical ASICs with unique functionality.

This material is covered by NDA between Sandia and Luxtera. If you are interested but not a Sandia employee, please contact the host (below).

CSRI POC: Erik DeBenedictis, (505) 284-4017

Title: Algorithms for LES in Complex Geometry

Speaker: Frank Ham, Stanford's ASC Center

Date/Time: Thursday, November 18, 2004, 9:00 - 10:00 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: As one of the five university alliances under the ASC program, Stanford's Center for Integrated Turbulence Simulations is using the ASC computers to simulate the complex flow and heat transfer through jet aircraft engines. These simulations tightly integrate two different codes running in different regions of the engine, each with different mathematical descriptions of the physics involved. The unsteady Reynolds-Averaged Navier Stokes (RANS) approach is being used for the trans-sonic flows and moving meshes of the compressor and turbine. In the combustor, the large eddy simulation (LES) approach is used because of its demonstrated superiority over RANS in predicting turbulent mixing, which is central to combustion.

In this seminar, Frank Ham will discuss center's development of algorithms suitable for LES in complex geometries, including the initial and largely unsuccessful effort to use staggered unstructured grids, and the details of the current control-volume based collocated finite volume formulation, where all discretization choices are made by considering their impact on secondary conservation

CSRI POC: Stefan Domino, (505) 284-4317 and Sheldon Tieszen, (505) 844-6526

Title: The Critical Role of Global Optimization in Computational Materials Science

Speaker: John Hamilton, Dept. 8761

Date/Time: Tuesday, September 14, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: My career at Sandia has included more than 10 years as an experimentalist and 10 years as a theoretician. During the years as a theoretician a common factor has emerged in a great number of the problems that I have worked on. That common factor is the necessity for better global optimization algorithms, which are readily accessible to the materials community.

In this talk I will present examples of materials problems, which require global optimization for their solution. These problems include surface alloys, structures of thin films and interfaces, structures of supported catalyst particles, and shapes of small precipitates in metals.

Because global optimization is a difficult problem, the average materials scientist tends to use relatively primitive techniques including simulated annealing, and local minimization from a large range of starting configurations commonly chosen based on experimental data.

With rapid increase in computer power and better algorithms for global optimization, substantial advances in computational materials science should be possible. I will discuss one possible approach to global optimization, which we are investigating, a combination of simulated annealing and accelerated molecular dynamics.

CSRI POC: John Aidun, (505) 844-1209

Title: Presentation from Linux Networx

Speaker: Joshua Harr and Scott Pearson, Linux Networx

Date/Time: Tuesday, February 10, 2004, 3:00-4:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Joshua Harr and Scott Pearson of Linux Networx will be making an NDA presentation covering Linux Networx's current and upcoming software technologies. Topics will include future storage solutions and just released cluster management technologies. Linux Networx will also discus their views and positions on the future of interconnects (including Infiniband), Open Source Software, and Linux distributions for HPC.

CSRI POC: Doug Doerfler, (505) 844-9528

Title: Branchwidth, Parallel Graph Algorithms, and Social Networks

Speaker: Dr. Illya Hicks, Texas A&M University

Date/Time: Monday, June 28, 2004, 10:00-11:00 am (PDST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: In this talk we introduce the notion of branchwidth and branch decompositions. We will explore basic definitions and methodologies associated branch decompositions and its possible usage in parallel graph algorithms and solving problems in social networks.

CSRI POC: Pamela Williams (925) 294-4683

Title: Exporting Parallel File Systems in a Scalable Manner with pNFS

Speaker: Dean Hildebrand, University of Michigan

Date/Time: Friday, August 6, 2004, 10:30-11:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Print, film, magnetic, and optical storage media produced about five exabytes of new information in 2002. Ninety-two percent of this information is stored on magnetic media, mostly in hard disks. Parallel file systems are the leading technology to provide scalable and secure access to this data, but limitations still exist. Parallel file systems are limited to a single operating system and do not interoperate with other file systems except through bandwidth limited technologies such as FTP and NFS. This talk presents the first implementation of Parallel NFS (pNFS), providing OS and file independent parallel file access while retaining all the benefits of NFSv4. The implementation exports the parallel file system PVFS2 and achieves throughput that approaches that of PVFS2 and dramatically better than NFSv4. This talk will present and discuss the pNFS implementation developed this summer at Sandia National Laboratories on the Linux platform.

CSRI POC: Sonja Tideman, (505) 284-0268

Title: Discrete Exterior Calculus: Applications in Mechanics, Computer Science and Applied Mathematics

Speaker: Anil Hirani, California Institute of Technology

Date/Time: Thursday, February 12, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: In this talk, intended for a general scientific audience, I will describe what exterior calculus is, how and why we discretized it, and place all this in the context of applications in computational mechanics and computer science. Calculus on nonlinear manifolds is the dominant language and tool of mechanics. This has been true at least since the work of Poincare, and to some extent even Euler and Lagrange. More recently, such a calculus is finding applications in computer science, statistics and applied mathematics. Exterior calculus is the technical name for this higher dimensional, nonlinear generalization of vector calculus. Identities of vector calculus have corresponding identities in exterior calculus. But exterior calculus is much richer, since nonlinear spaces can have a much richer structure than linear spaces.

This rich structure, when exploited in computations, can lead to structure preserving, stable numerical methods for computational mechanics, as well as provide solutions for many problems in computer science. In computational electromagnetism, the success of edge-elements, pioneered in part by Alain Bossavit, shows a glimpse of what is possible. The work by various people in computational electromagnetism and in theoretical physics, was the start of discretization of small parts of exterior calculus for specific applications. In my thesis, I took on the task of a systematic discretization of exterior calculus. At the same time, with some collaborators, I have been experimenting with applications like thin shell dynamics and other problems in elasticity, vector field decomposition, nonlinear waves, and image analysis.

CSRI POC: Pavel Bochev, (505) 844-1990

Title: "Consider a Spherical Cow" -- Conservation of Geometry in Analysis: Implications for Computational Methods in Engineering

Speaker: Dr. Thomas J. R. Hughes, University of Texas, Austin

Date/Time: Monday, June 14, 2004, 1:00-2:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: "Consider a spherical cow" is the punch line of a mathematics joke. The joke itself is not so important to the subject of this work but the message is, namely, that simplifications of geometry are often made to facilitate analysis. Let us take the engineering design process as an example. There are estimated to be of the order of a million analyses a day performed in engineering design offices throughout the world. Engineering designs are encapsulated in Computer Aided Design (CAD) systems. Up to manufacturing tolerances, these systems exactly represent the geometry of designs. The analysis process begins with CAD geometry but the predominate method of analysis, finite elements, requires a different representation of geometry. This creates two problems: 1) The need to generate the geometric description suitable for the finite element method; and 2) the geometric errors that are produced in the process. The first problem, "mesh generation," is attributed to taking over 80% of all analysis time in major engineering industries such as shipbuilding, aerospace and automotive. It has become the major bottleneck in engineering analysis. The second problem is very important in certain situations, such as, for example, the buckling of thin shells, which exhibit strong geometric imperfection sensitivity. Since approximating the geometry for analysis purposes is costly, time consuming, and potentially creates significant errors, it raises the question, why do we do it? It would seem beneficial to conserve the exact CAD geometry in analysis, up to, of course, features that we definitely want to remove. This work takes the point of view that conserving geometry is an important conservation law that should be satisfied. We pursue this idea and see where it takes us. It suggests a very different analytical structure but one in which mesh generation may be dramatically simplified. Some simple computations in structural analysis are presented which indicate the ideas are viable and we argue why we feel that developing a complete mathematical convergence theory may be straightforward.

CSRI POC: Scott Collis, (505) 284-1123

Title: Multiscale Methods for Flows with Moving Boundaries

Speaker: Steven Hulshoff, Delft University of Technology

Date/Time: Thursday, December 2, 2004, 1:00 pm – 2:30 pm

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: Several challenging problems in aerospace engineering, such as the design of flow-control systems and the prediction of aeroelastic phenomena, require accurate descriptions of the behavior of turbulent flows near moving boundaries. A promising approach is based on the unification of variational-multiscale (VMS) techniques for large-eddy simulation with finite-element methods (FEM). VMS techniques can provide superior predictions of large-scale functionals due to their consistency with the governing equations at large scales. When implemented within finite-element methods, VMS techniques can also be applied to complex geometries, and be naturally incorporated into h-p adaptive solution procedures.

There are several approaches, however, to the implementation of VMS-FEM. In this talk, three VMS space-time finite-element discretizations are compared. The first is based on the modal spectral-element method, the second on the partition-of-unity concept, and the last on the discontinuous-Galerkin method. Their performance is evaluated using one-dimensional viscous Burgers computations, which allows subgrid-scale modeling parameters to be clearly identified. The effects of mesh refinement, number of scales and scale partitioning on solution accuracy are illustrated.

As for traditional methods, the near-wall resolution requirements of VMS-FEM large-eddy simulations become prohibitive at high Reynolds numbers. There is therefore substantial motivation to develop hybrid techniques which make use of Reynolds-averaged models in the immediate vicinity of walls. In the second part of the talk, a new multiscale method for combining VMS-LES with Reynolds-averaged methods is presented. The latter avoids some of the boundary condition and modeling problems encountered in existing hybrid techniques.

CSRI POC: Scott Collis, (505) 284-1123

Title: Water and protons in narrow molecular pores: from nanotubes to proteins

Speaker: Gerhard Hummer, U.S. Dept. of Health & Human Services

Date/Time: Friday, April 2, 2004 - 1:30-2:30 pm

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: Water exclusion from the hydrophobic core is a paradigm of protein stability. Protein function, in contrast, often requires water penetration into the nonpolar interior. Biomolecular proton conduction occurs through transiently solvated hydrophobic channels, as in the proton pumps cytochrome c oxidase and bacteriorhodopsin. Water itself is selectively transported across biological membranes through predominantly hydrophobic, not hydrophilic channels, as in aquaporin-1. Why do water molecules occupy such narrow hydrophobic channels where they can form only few hydrogen bonds, and thus lose many kT in energy compared to bulk solution? How do water molecules get into, through, and out of such hydrophobic channels? An analysis of the water, proton, and solute transport through the simplest molecular hydrophobic channel, a carbon nanotube, addresses these questions and sheds new light on the functional role of hydrophobic channels in proteins for water and proton transport. Molecular dynamics simulations show that nanotubes in contact with a water reservoir can fluctuate in sharp transitions between water-filled and empty states. In the filled state, water molecules move rapidly and in a highly concerted fashion through the sub-nanometer pores. An osmotic setup will be used to study the nearly frictionless nanoscale flow through nanotubes assembled into membranes, and to characterize the properties of two-dimensionally confined water monolayers that form between the nanotube membranes. Transport of small hydrophobic molecules through nanotubes illustrates how selective binding leads to selective transport of low-concentration solutes. Simulations with Car-Parrinello molecular dynamics and an empirical valence bond model for water show that the one-dimensionally ordered water chains spanning the nanotube pores provide excellent "proton wires" with forty-fold higher single-proton mobilities than bulk water. These results have important implications for the transfer of water and protons through proteins and across membranes in biological systems. In particular, they lead to a detailed molecular model of the proton-pumping mechanism of cytochrome c oxidase that explains how this biological "fuel cell" can power aerobic life by exploiting the unique properties of confined water.

CSRI POC: Susan Rempe, (505) 845-0253

Title: The Interplay of Ca2+ Dynamics and Ryanodine Receptor Distribution Influences Ca2+ Wave Propagation in Atrial Myocytes

Speaker: Leighton Izu, University of Maryland

Date/Time: Tuesday, February 24, 2004, 2:00-3:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Mathematical modeling has shown that the distribution of ryanodine receptors (RyRs, the calcium release channel) in atrial cells is critically important for the initiation and propagation of calcium (Ca2+) waves. We investigated the effect of RyR spacing in the plane of the z-line on model behavior and demonstrate a surprisingly strong coupling between the mechanics of contraction and the Ca2+ control dynamics. (1) Previous studies suggest that the RyR spacing in the transverse direction, is 2 (m. However, our simulations showed that Ca2+ waves could not occur with this large a spacing using realistic model parameters but could occur if were ~1 (m. We tested this prediction by measuring the distances between fluorescently tagged antibodies to RyR with a confocal microscope. We found that =0.8 (0.3 (m consistent with the model prediction. (2) Antibody labeling experiments also revealed the presence of RyRs interspersed about halfway between z-lines (mean spacing between RyRs on periphery = 0.9 (0.4 (m) on the surface sarcolemma but not in the cell interior. Simulations show that the higher packing density of RyRs on the sarcolemma will result in a transverse gradient in the longitudinal Ca2+ wave velocity. This gradient becomes more pronounced under conditions where Ca2+ wave propagation is not robust (low Ca2+ load in the sarcoplasmic reticulum, low Ca2+-sensitivity of the RyRs). (3) The typical diastolic sarcomeric spacing of RyR is 2 (m but can be smaller when resting Ca2+ is elevated such as during heart failure. We found that modest reductions of~10-20% in the longitudinal spacing of the RyRs, caused a tremendous 5- to 30-fold increase in the probability of Ca2+ wave initiation, profoundly increasing the likelihood of spontaneous Ca2+ waves. Because spontaneous Ca2+ waves can trigger arrhythmias we propose that changes in the geometry of RyR distribution may play an important role in arrhythmogenesis common during heart failure.

CSRI POC: Shawn Means, (505) 844-1699

Title: Continuation Algorithms for Parameter Dependent Compact Fixed Point Problems

Speaker: Prof. C. T. Kelley, North Carolina State University

Date/Time: Tuesday, June 22, 2004, 10:00-11:00 am (PDST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: In this talk we show how compactness can be used to design and analyze Newton-Krylov and multilevel algorithms for parameter-dependent compact fixed-point problems. Such problems arise not only as integral equations, but also from indirect integrations such as source iteration in radiative transfer calculations and time-stepping approaches to dynamic analysis of parabolic partial differential equations.

The methods we propose are easy to implement and require no detailed knowledge of the internal structure of the fixed-point map. We will illustrate the ideas with examples from integral equations and dynamic analysis.

CSRI POC: Tammy Kolda, (925) 294-4769

Title: Solving and Analyzing Side-chain Positioning Problems Using Linear and Integer Programming

Speaker: Carl Kingsford , Princeton University

Date/Time: Tuesday, August 10, 2004, 1:00-2:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Determining the positions of a protein's side chains is a central step in homology modeling and protein design. In a common formulation of the problem, the backbone is fixed, side-chain conformations come from a rotamer library, and a pairwise energy function is optimized. It is NP-complete to find even a reasonable approximate solution.

We introduce a new integer linear programming formulation of side-chain positioning that allows us to tackle large problem sizes. We relax the integrality constraints to give a polynomial-time linear programming (LP) heuristic and apply LP to position side chains on native and homologous backbones and to choose side chains for protein design.

We present the first large-scale demonstration that LP-based approaches are highly effective in finding optimal (and near-optimal), accurate solutions for the side-chain positioning problem. Surprisingly, when positioning side chains on native and homologous backbones, optimal integral solutions for a simple, biologically meaningful energy function can usually be found using LP. Design problems often cannot be solved using LP directly, but optimal solutions for large instances can still be found using the computationally more expensive integer linear programming formulation.

This is joint work with Bernard Chazelle and Mona Singh.

CSRI POC: Bill Hart, (505) 844-2217

Title: Uniform Finite Element Error Estimates for Differential Equations with Jumps in Coefficients

Speaker: Andrew Knyazev, University of Colorado, Denver

Date/Time: Wednesday, August 18, 2004, 10:00-11:00 am

Location: Building 980 Room 24 (Sandia NM)

Brief Abstract: We consider a parametric family of boundary value problems for the diffusion equation with the diffusion coefficient equal to a small constant in a subdomain. Such problems are not uniformly well posed when the constant gets small. However, in a series of papers, Bakhvalov and Knyazev have suggested a natural splitting of the problem into two well-posed problems. Using this idea, we prove a uniform regularity of the solution and a uniform finite element error estimate for our model problem in the standard parameter-independent Sobolev norm. We consider a traditional finite element method with only one additional assumption, namely, that the boundary of the subdomain with the small coefficient does not cut any finite element.

The talk is based on a joint paper with Olof Widlund, Lavrentiev Regularization + Ritz Approximation = Uniform Finite Element Error Estimates for Differential Equations with Rough Coefficients. Mathematics of Computation, 72 (2003).

CSRI POC: Rich Lehoucq, (505) 845-8929

Title: Modeling nitric oxide release from nitrophorin

Speaker: Dmitry Kondrashov (Post Doc Candidate), University of Arizona

Date/Time: Tuesday, November 16, 2004, 10:30-11:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: The nitric oxide (NO) transport protein nitrophorin is able to modulate NO release rates by two orders of magnitude in response to pH change, and the rates are much slower than in the classic transport protein myoglobin. Experiments have shown that a large conformational change in two loops near the heme binding site is apparently reponsible for controlling NO release. We study this mechanism using atomic-resolution X-ray crystallography, stochastic modeling, and molecular dynamics simulations. Crystal structures reveal that the key loops exhibit a mixture of conformations under all the conditions studied, suggesting that the loops are not a static barrier to NO escape. We base a stochastic model on these observations, by modeling the loops as a fluctating gate and NO as a diffusing particle inside the protein, where it can rebind to the heme or escape out of the protein. We present an analytical solution of NO escape rates as a function of loop opening and closing rates, and find that in the appropriate regime there are two different slow rates, consistent with experiments, one of which depends on the opening rate and one on the probability of rebinding. We also perform molecular dynamics simulations to observe NO migration as a function of protein conformation. The simulations agree closely with the X-ray structures, and allow us to observe NO migration and escape into the solvent. In contrast to myoglobin, nitrophorin does not allow NO migration into internal protein cavities, which enhances the probability of NO rebinding to the heme, and, as predicted by our model, leads to dramatically slower NO release rates in nitrophorin compared to myoglobin.

CSRI POC: Mark D. Rintoul, (505) 844-9592

Title: Residual-Based Error Estimation for Lagrangian Hydrocodes

Speaker: Marc LaForest, Ecole Polytechnique de Montreal

Date/Time: Wednesday, December 1, 2004, 9:00 - 10:00 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: There is a long history of using Lagrangian hydrocodes for the simulation of compressible gas dynamics. Unfortunately, despite their widespread use and their speed, there are no effective means of estimating the error in their simulations. Besides providing a means for code verification, the error estimators could be used for the adaptive control of the mesh, of the order of the scheme, and potentially even of the underlying physical model. Most error estimation techniques for time-dependent problems are difficult, if not impossible, to apply to Lagrangian approximations. Hydrocodes are therefore limited to gradient and jump indicators.

The object of this presentation is to review work that has been done towards building an inexpensive and local error estimator that could be implemented directly into existing hydrocodes. We present two error indicators. The first, based on a smoothness indicator of Karni, Kurganov, and Petrova, is an evaluation in weak form of the residual. The second is constructed by combining a piecewise linear reconstruction of density and pressure with an approximate solution of the error equation in the space of continuous piecewise quadratic polynomials. The second estimator is related in part to work of Oden and Prudhomme. We discuss mathematical and numerical issues in the implementation of these error indicators and present results showing their reliability, cost, and range of application.

CSRI POC: Thomas Voth, (505) 844-6004

Title: Performance Analysis of a Chosen Workload to Represent Sandia National Laboratories' Scientific Applications

Speaker: Charles Laverty, New Mexico State University (student intern)

Date/Time: Wednesday, August 11, 2004, 10:00-11:00 am

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: A test workload provided by FEI (Finite Element Interface) called cube3.exe, which is an abstraction layer between applications and solver libraries, has been used as the test driver for a uni-processor performance study for SNL's scientific-computing applications. From the use of hardware counters on the Itanium 2 processor and output from the Sim-Alpha simulator (validated Alpha 21264 simulator) various characteristics and performance measures of the cube3.exe workload will be presented. Also, using a modified version of the Sim-Alpha simulator, sensitivity analysis has been performed by varying architecture structure sizes to determine optimum processor characteristics for future complex computing. Performance of CTH as the problem is divided among processors will also be shown.

CSRI POC: Erik DeBenedictis, (505) 284-4017

Title: Induction of Interleukin 6 and Interleukin 15 by Salmonella Enterica Serovar Typhimurium in Calves

Speaker: Sara D. Lawhon, Texas A&M University

Date/Time: Wednesday, August 4, 2004, 10:00-12:00 pm (MDST)

Location: Building 980 Room 95 (Sandia NM)
Building MO52 Room 165 (Sandia CA)--videoconference

Brief Abstract: Background: Salmonella is the leading cause of death due to food-borne illness in the United States. Salmonella enterica Serovar Typhimurium (hereafter S. typhimurium) is the most commonly isolated Salmonella serovar from these cases. S. typhimurium causes enterocolitis in humans, which is characterized by inflammation, polymorphonuclear cell (PMN) infiltration of the intestine, and diarrhea. Experimental infection of calves and non-human primates with S. typhimurium results in pathological changes Similar to those found in human cases including PMN infiltration and fluid secretion. Previous studies in our laboratory confirmed the role of S. typhimurium effectors SipA, SopA, SopB, SopD and SopE2, in fluid secretion, PMN infiltration, and expression of CXC chemokines in the bovine ligated ileal loop model. Interleukin 6 (IL-6) has been implicated in enhanced phagocytosis and killing of S. typhimurium by PMN. Interleukin 15 (IL-15) has been described as an intestinal epithelial growth factor and is involved in PMN secretion of IL-8.

Methods: We investigated the role of S. typhimurium effectors SipA, SopA, SopB, SopD and SopE2, in the induction of IL-6 and IL-15 by real time PCR in bovine ligated ileal loops. Briefly, ligated ileal loops were inoculated with sterile LB broth, wild type S. typhimurium, or a S. typhimurium strain carrying mutations in sipA, sopA, sopB, sopD, and sopE2 (sipAsopABDE2 mutant). Fluid and tissue samples were collected for histopathology, RNA extraction, and bacterial enumeration at time points between in the LB loops. Significantly less fluid was present in the loops inoculated with the mutant as compared to loops inoculated with wild type. IL-6 and IL-15 expression was increased, particularly IL-6, in loops inoculated with either wild type S. typhimurium or sipAsopABDE2 mutant but not in loops inoculated with Luria-Bertani broth.

Conclusion: The in vivo model of bovine ligated ileal loop suggests that expression of IL-6 and IL-15 cytokines is independent of SPI-1 mediated invasion.

CSRI POC: George S. Davidson, (505) 844-7902

Title: High Fidelity Simulations in Reactive Flows: the role of chemical kinetics and model reduction

Speaker: Jeremiah C. Lee, SNL CA

Date/Time: Wednesday, October 6, 2004, 9:30-10:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: High fidelity simulation of reactive flows has carved a niche for itself in basic combustion research in the past two decades. Progressively, its role expands and evolves from being an accompaniment to various ``standard'' reference flame experiments to being one of the mainstream tools to generate data for flame dynamics research. The intrinsic value of this kind of simulations lies not only in the amount of otherwise unobtainable detail information on the flame structure and its dynamical behavior, but also in the massive data base they generate for model reduction and validation. This is particularly important for systems that involve large kinetic mechanisms; and one should also keep in mind that combustion is not the only field, which involves large and stiff kinetics. A key factor and challenge in the future advancement of this field is the construction of an accurate model that has an extended range of applicability.

In the two parts of this talk, I shall first discuss the classic application of high fidelity simulations; such as particle combustion, the flame-vortex numerical experiments, and a study on edge flames. This will be followed by a discussion on the construction of reduced models. We will concentrate on a singular perturbation based algorithm, which enables the construction of an adaptive chemistry model. This new algorithm may even change fundamentally the way to handle the stiff chemical source term in large scale simulations.

CSRI POC: John Shadid, (505) 845-7876

Title: Broken Symmetries: Why is there so much matter in the universe, and how can the BaBar experiment shed light on this question?

Speaker: Vincent (Bram) Lilliard, University of Maryland

Date/Time: Thursday, January 22, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: The symmetry between matter and anti-matter pervades our understanding of fundamental particle interactions. However, current observation reveals a matter-dominated universe, requiring a better understanding of both the Big Bang theory and the Standard Model of particle physics. The combined symmetry of charge conjugation (C) and parity (P) is violated in B meson decays. This elusive phenomenon, called "CP violation", was observed in neutral kaon decays in 1964, but was the only experimental evidence of a particle-antiparticle asymmetry prior to recent results from the BaBar experiment at the Stanford Linear Accelerator Center (SLAC). Theories predict large CP violating asymmetries in B decays but do not provide a large enough effect to explain the matter-antimatter asymmetry observed in cosmological data. Thus, an effort to measure this effect could provide confirmation of the Standard Model and/or a glimpse of physics not yet observed or understood. This presentation will introduce the concepts of fundamental particle physics which gives rise to the current understanding of CP violation, as well as the motivation and recent experimental results from the BaBar collaboration at SLAC.

CSRI POC: David Womble, (505) 845-7471

Title: A Compiler-Based Approach to Specializing Software Libraries

Speaker: Calvin Lin, University of Texas at Austin

Date/Time: Monday, January 12, 2004, 11:00 – 12:00 noon (MT)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: Software libraries are a popular means of re-using code. Unfortunately, the static black-box nature of libraries can thwart compiler optimizations, limit code reuse, and threaten portability. This talk introduces a compiler-based approach to optimizing both software libraries and the application programs that use them. The key is a simple annotation language that describes semantic information about libraries. The result is a compiler that can analyze and transform library operations in the same way that language primitives can be analyzed and transformed. Experiments with the PLAPACK parallel linear algebra library show that this technique can yield significant performance improvements, even for a library that has been carefully designed to provide good performance.

CSRI POC: Patty Hough, (925) 294-1518

Title: Towards Bootstrap Algebraic Multigrid (BAM)

Speaker: Oren Livne, Stanford University

Date/Time: Wednesday, March 10, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: Multigrid methods have solved many problems, with the amount of computational work being proportional to the amount of real physical changes in the computed system. However, complicated applications and geometries require expertise and complex programming, if at all possible. Thus, Algebraic Multigrid (AMG) solvers were developed, based on multigrid principles, without explicitly using the geometry of the grids in the problem. AMG is a robust black-box solver for large sparse linear systems of equations, usually arising from second-order elliptic PDEs. It might constitute the "next generation" of multigrid, but its scope is still rather limited to such problems. The goal of this work is to extend AMG: to general non-scalar, or high-order, or non-elliptic, or anisotropic PDE systems, and also for non-variational discretizations. The new method is called Bootstrap Algebraic Multigrid (BAM), because it is based on a self-correction principle: given a current solver, we find the slow-to-converge errors, and adapt the solver to them. This process is repeated until a fast solver emerges. The talk concerns BAM's two main parts: (a) We discuss three problems related to automatically generating and assessing the quality of coarse "grids" in BAM, and their solution. The process of constructing the coarse grid is self-corrective, based on Compatible Relaxation (CR). We will present some theory, an algorithm, and numerical results for model problems. (b) We also outline the construction of accurate inter-grid transfer operators, which is still under investigation. Once this challenging "missing link" is well understood, it will be possible to construct the entire BAM solver, and test it against problems that are beyond the scope of AMG.

CSRI POC: Jonathan Hu, (925) 294-2931

Title: Periodic Solutions of Chaotic Partial Differential Equations

Speaker: Vanessa Lopez, Interview Candidate, University of Illinois at Urbana-Champaign

Date/Time: Wednesday, July 14, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: We consider the problem of finding relative time-periodic solutions of chaotic partial differential equations with symmetries. Relative time-periodic solutions are solutions that are periodic in time, up to a transformation by an element of the equations' symmetry group. As a model problem we work with the 1D complex Ginzburg-Landau equation (CGLE), which is a standard example of an evolution equation that exhibits chaotic behavior. The problem of finding relative time-periodic solutions numerically is reduced to one of finding solutions to a system of nonlinear algebraic equations, obtained after applying a spectral-Galerkin discretization in space and time to the CGLE. The discretization is designed to include as an unknown the group element that defines a relative time-periodic solution. Using this approach, we found a large collection of distinct relative time-periodic solutions in a chaotic region of the CGLE. These solutions, all of which have broad temporal and spatial spectra, were previously unknown. There is a great deal of variety in their Lyapunov spectra and spatio-temporal profiles. Moreover, none bear resemblance to the time-periodic solutions of the CGLE studied previously. We also consider the Navier-Stokes equations for an incompressible fluid and present preliminary work towards the problem of finding relative time-periodic solutions of these equations.

CSRI POC: John Shadid, (505) 845-7876

Title: Periodic Solutions of Chaotic Partial Differential Equations

Speaker: Vanessa Lopez, Interview Candidate, University of Illinois at Urbana-Champaign

Date/Time: Friday, September 24, 2004, 10:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: He will talk about his work on ab initio molecular dynamics of water and the DFT-MC technique (sampling molecular configuration at finite temperature using Monte Carlo and density functional theory energy landscape). His seems to be on vacation, and it is unlikely we will send out a title and abstract until the week of 9/21. However, the talk will likely address the very current issues of the recent controversy of ab initio molecular dynamics of water, as well as the prospect of computing phase diagrams and phase boundaries using DFT-MC techniques.

CSRI POC: Vitus Leung, (505) 844-1896 and Marcus Martin, (505) 284-6355

Title: Fast Monte Carlo Algorithms for Matrix Operations and Massive Data Set Analysis

Speaker: Michael W. Mahoney, Yale University

Date/Time: Thursday, September 16, 2004
10:00 – 11:00AM (PDST)
11:00 – 1200 Noon (MDST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: We are interested in developing and analyzing fast Monte Carlo algorithms for performing useful computations on large matrices. Examples of such computations include matrix multiplication, the computation of the Singular Value Decomposition of a matrix, the computation of the compressed approximate CUR decomposition of a matrix, and testing the feasibility or infeasibility of a linear program. We present a Pass-Efficient model of data streaming computation in which our algorithms may naturally be formulated and present algorithms that are efficient within this model for each of the four types of matrix operations mentioned previously. We then describe how extensions of the CUR decomposition may be used for improved kernel-based statistical learning and for the efficient approximation of massive tensor-based data sets.

This is joint work with Petros Drineas and Ravi Kannan.

CSRI POC: Monica Martinez-Canales, (925) 294-3157

Title: Computational Modeling of the Mechanical Behavior of Metals

Speaker: Antoinette Maniatty, Department of Mechanical, Aerospace, and Nuclear Engineering,, Rensselaer Polytechnic Institute

Date/Time: Monday, June 21, 2004, 2:00-3:00 pm (MDST)

Location: Building 980 Room 95 (Sandia NM)
Building 916 Room 101 (Sandia CA)--videoconference

Brief Abstract: This talk will consist of two parts. In the first part, an efficient, stabilized, finite element formulation for modeling large, elastic-plastic deformations at the macroscale will be presented. The advantages of this formulation are that it:

(a) Circumvents the Babuska-Brezzi condition providing freedom in choosing interpolation functions,
(b) Avoids mesh locking and spurious pressure modes,
(c) Enhances stability in the presence of incompressibility, and
(d) Allows efficient, low-order P1/P1 elements (linear interpolation for both the displacement and pressure) with fewer degrees of freedom for similar accuracy compared to an a priori stabile finite element (satisfying the Babuska-Brezzi condition).

In the second part, work on multi-scale modeling of polycrystalline, metallic materials is presented. In this work, the focus is at the grain scale. Material models at this scale are based on dislocation phenomena occurring at the smaller scale. The grain scale model is linked to the larger scale either through a grain interaction law leading to an averaging procedure or through a representative volume element with appropriate periodic boundary conditions.

Examples involving metal forming and the mechanical behavior of polycrystalline thin films will be presented to demonstrate each algorithm.

CSRI POC: Scott Collis, (505) 284-1123

Title: Vorticity structure and evolution in a transverse jet with new Algorithms for scalable particle simulation

Speaker: Youssef Marzouk (Truman Fellowship Candidate), Massachusetts Institute of Technology

Date/Time: Wednesday, April 7, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 916 Room 101 (Sandia CA)--videoconference

Brief Abstract: Transverse jets enjoy a wide range of engineering applications, from propulsion and power generation to exhaust dispersion. This study seeks a mechanistic understanding of vorticity structure and evolution in the transverse jet in order to develop actuation strategies that manipulate the geometry and rate of mixing between jet and crossflow.

We develop a massively parallel 3-D vortex element simulation of a transverse jet at high Reynolds number. A new formulation of vorticity flux boundary conditions enables several modes of jet actuation to be studied computationally. Simulations of the unforced transverse jet reveal mechanisms by which coherent vortical structures are formed, a process that previously has not been well understood. In particular, we analyze the coupling between the initiation of a counter-rotating vortex pair and the folding of ring-like vortical structures downstream of the jet exit. Current work examines the role of these vortical structures in mixing and their response to actuation. Dynamical systems techniques are used to identify coherent structure boundaries that organize finite-time mixing. An analytical description of vortex filament geometry in the near field of the jet shows dependence on parameters that describe unsteady actuation at the jet nozzle.

A complementary component of this work focuses on algorithms for massively parallel simulation. We introduce new clustering methods for parallel domain decomposition of N-body interactions, examining the optimality of the resulting cluster geometries and demonstrating heuristics for dynamic load balancing. These tools are applicable to parallel simulation of N-body problems in a variety of fields.

CSRI POC: Sudip Dosanjh, (505) 845-7018
Andrew Salinger, (505) 845-3523
Larry Rahn, (925) 294-2091

Title: Large Graphs from the Real World

Speaker: Kevin McCurley, IBM Almaden Research Center

Date/Time: Thursday, September 2, 2004, 10:00-11:00 am (MDT)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: There are many examples of large data sets in the real world with intrinsic mathematical structure of a graph. Two examples are the hyperlink structure of the World Wide Web, and the relationship structure of social networks. The ability to collect such data on a massive scale has resulted in a great deal of activity on mathematical modeling and algorithms for large graphs. For example, at IBM Almaden we have been crawling and collecting a copy of the World Wide Web that now contains billions of nodes and tens of billions of edges. In this talk I will describe some characteristics of such graphs, as well as some algorithmic problems that have emerged from attempts to extract value from the web and social network graphs. Among other things, these problems have applications to homeland security.

CSRI POC: Bruce Hendrickson, (505) 845-7599

Title: Simulation of Twinned-Martensite as a PDE Optimization Problem

Speaker: Luis A. Melara and Anthony J. Kearsley, National Institute of Standards and Technology

Date/Time: Monday, June 7, 2004, 10:00-11:00 am (MDT)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: Developing numerical methods for predicting microstructure in materials is an extremely large and important research area. Two examples of material microstructures are Austenite and Martensite. Austenite is a microscopic phase with simple crystallographic structure while Martensite is one with a more complex structure. One important task in materials science is the development of numerical procedures which accurately predict microstructures in Martensite near an Austenite-twinned-Martensite interface. In this talk we present two numerical approaches: one that involves the solution to an equality constrained optimization problem and a second that requires the solution to an inequality constrained optimization problem. Numerical methods for solving both problems are presented together with a computationally affordable way of approximating the inequality constraint that appears in our second problem formulation. Preliminary results suggest that the minimizers of the constrained optimization problems display desirable characteristics.

CSRI POC: Paul Boggs, (925) 294-4630

Title: Dynamic Metadata Management for Large-Scale File Systems

Speaker: Ethan L. Miller, University of California, Santa Cruz

Date/Time: Tuesday, August 17, 2004, 10:00-12:00 noon

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: In pet byte-scale distributed file systems that decouple read and write from metadata operations, behavior of the metadata server cluster is critical to overall system performance and scalability. This talk will present a dynamic sub tree partitioning and adaptive metadata management system designed to efficiently manage hierarchical metadata workloads that evolve over time. This approach is compared via simulation to other metadata partitioning strategies such as sub tree partitioning and hashing, demonstrating the performance, scalability, and adaptability advantages.

This is joint work with Sage Weil, Krista Pollack, and Scott Brandt, and was conducted at the Storage Systems Research Center at the University of California, Santa Cruz.

CSRI POC: Ron Oldfield, (505) 284-9153

Title: Exploiting Kronecker Product Structure in Image Restoration

Speaker: Professor James G. Nagy, Emory University

Date/Time: Wednesday, February 4, 2004, 10:00-11:00 am (PT)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--Videoconference

Brief Abstract: Image restoration is the process of minimizing or removing degradations from an observed image, which may be distorted by such things as blurring and noise. Such problems arise in applications ranging from microscopy to astronomy. Computational methods for restoring the image require solving large, very ill-conditioned linear systems. The structure of the "blurring" matrix determines whether it is feasible to use matrix factorizations, or whether iterative methods are more appropriate for solving the linear systems. In this talk we describe some aspects of image restoration algorithms, and show that the blurring matrix can often be represented in terms of Kronecker products. We also show how to exploit the Kronecker product structure to improve computational efficiency. Examples from various applications will be presented.

CSRI POC: Tammy Kolda (925) 294-4769

Title: Techniques for Solving Equations Arising from Nonlinear Finite Element Analysis

Speaker: Michael L. Parks, University of Illinois at Urbana-Champaign

Date/Time: Thursday, April 29, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)—videoconference

Brief Abstract: Research on failure mechanisms (e.g. fatigue and fracture) of engineering components often focuses on modeling complex, nonlinear response. The analysis by finite element methods requires large-scale, very refined 3D solid models. Domain decomposition methods are frequently employed. Finite element methods for quasi-static and transient responses over longer time scales generally adopt an implicit formulation. Together with a Newton scheme for the nonlinear equations, such implicit formulations require the solution of large linear systems, thousands of times, to accomplish a realistic analysis. This represents an enormous computational burden.

To reduce the overall solution time for a sequence of linear systems, we must develop more intelligent Krylov subspace methods. Linear solvers that retain a subspace determined while solving previous systems can use that subspace to reduce the cost of solving the next system in the sequence. We refer to this process as *Krylov subspace recycling*. I discuss two different approaches, and demonstrate on a model problem that we can reduce the iteration count required to solve a linear system by a factor of two.

Improved domain decomposition methods can also lessen the computational costs. We consider the finite element tearing and interconnecting (FETI) method, as it is among the most popular domain decomposition methods, and shows both numerical and parallel scalability. Application of the one-level FETI method produces a KKT (Karush-Kuhn-Tucker) linear system. Existing FETI preconditioners are generally based on mechanical arguments about the system being solved. I approach the FETI dual interface problem from a purely algebraic viewpoint, and connect existing KKT preconditioners to FETI preconditioners. This algebraic connection allows analysis of the FETI method from a new perspective, and suggests potential improvements.

CSRI POC: Rich Lehoucq, (505) 845-8929

Title: Communicationless Parallel Mesh Refinement

Speaker: Philippe P. Pebay, Org. 8351, Reacting Flow Research

Date/Time: Tuesday, September 14, 2004, 10:30 – 11:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: This talk will present a new technique for the parallel adaptive refinement of tetrahedral meshes. This technique is new because no neighbor information is required for the refined mesh to be compatible everywhere. That feature makes it especially suitable for parallel mesh refinement.

Refinement consists of inserting new vertices at edge midpoints until some tolerance (geometric or otherwise) is met. For a tetrahedron, the six edges present 2^6=64 possible subdivision combinations. The challenge is to triangulate the new vertices (i.e., the original vertices plus some subset of the edge midpoints) in a way that neighboring tetrahedra always generate the same triangles on their shared boundary. A geometric solution based on edge was developed previously, but did not account for geometric degeneracies (edges of equal length). This talk will provide a solution that lifts such ambiguities without communication between neighboring elements.

Due to the large number of possible geometric configurations, implementation was not trivial. We have therefore developed a Python C++ code generator based on the permutations of the symmetric group of order 4. This has allowed us to generate the subdivision code from a much smaller number of "canonical" cases. This talk will explain our code generation method, since it could also be used for other applications.

Finally, this talk will analyze the performance of the technique by characterizing mesh quality, execution time, and traits of the algorithm that could affect quality or execution time differently for different meshes.

CSRI POC: Richard Lehoucq, (505) 845-8929

Title: Solution Verification in Computational Mechanics via Certificates

Speaker: Jaime Peraire, Massachusetts Institute of Technology

Date/Time: Wednesday, June 9, 2004, 2:00-3:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Approximations to the solutions of Partial Differential Equations are computed routinely in engineering design and practice. Even for the simplest and best-studied equations such as elasticity, heat transfer or convection-diffusion, the accuracy of the computed results cannot be rigorously guaranteed in general situations. The reasons are twofold: first, existing algorithms for error estimation contain constants or parameters which are ambiguous and result in uncertain results, e.g. continuity constants, reference meshes, numerical integration of analytic functions etc.; second, algorithms are implemented in computer codes which may contain thousands and even millions of lines which are virtually impossible to verify in a rigorous manner.

We propose the idea of a certificate for the solution of PDE. A certificate consists of a stand-alone data set that can be used to document and to prove the correctness of a given claim. Exercising the certificate is done by means of a simple algorithm, in fact much simpler than that used to compute it, and more importantly, it can be done a-posteriori and without recourse to the computer code or algorithms used to generate it. We certify upper and lower bounds for functional outputs of the exact solutions of partial differential equations. We note that the length, or size, of the certificate depends on the bound gap. In the presentation we will concentrate on describing such certificates, and providing some algorithms to adaptively compute them for a prescribed level of accuracy. Our focus will be on outputs of engineering interest such as displacements, collapse loads or heat fluxes. We will present results for both linear and non-linear equations, including the equations of elasticity, convection-diffusion and limit analysis; as well as linear an non-linear outputs of the solution, such as forces, displacements or energy release rates.

CSRI POC: Jim Stewart, (505) 844-8630

Title: A Parallel Algorithmic Approach to Characterize and Optimize Stable Clusters and Cores

Speaker: Stefan Pickl, University of Cologne

Date/Time: Thursday, April 29, 10:00-11:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: This talk will give an introduction to the challenging field of the optimization of biosystems and economic systems by applying discrete structures and suitable algorithms. Many optimization problems can be described and solved with the aid of polytopes by exploiting their geometrical and combinatorial structure. The presentation describes two cases where polytopes determine feasible sets: economathematics and data analysis in the lifesciences. In particular we will consider the computation of stable time-series experiments to analyze clusters in DNA. In these fields, our algorithms use a special polytope representation to analyze and optimize a nonlinear time-discrete system. The underlying theory of the algorithm is based on the use of polytopes and linear programming techniques that successively examine only the extremal points of the polytope. We present theoretical and numerical results. In particular this technology is used in project TEMPI (Technology Emissions Means Process Identification), a nonlinear discrete-time economic model which has been applied to environmental management problems.

CSRI POC: Cindy Phillips, (505) 845-7296

Title: Research Projects Ongoing at the Bioinformatics Center at NMSU

Speaker: Desh Ranjan and Jing He, New Mexico State University

Date/Time: Monday, November 29, 2004, 10:30-11:30 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: In this talk, Dr. Desh Ranjan will give an introduction of the newly established center at NMSU - Center for Research Excellence in Bioinformatics and Computational Biology that was recently funded by NSF. Particularly, he will discuss the four research projects currently conducted in this center. Dr. Ranjan's primary interest is in efficient algorithm design in computational biology. He has been involved in designing sequential and parallel algorithms for calculating solvent accessible surface area for proteins. Dr. Jing He will discuss her project of deriving 3-dimensional protein structure using constraints in the protein density map at intermediate resolution. A parallel algorithm for building a library of possible assignments for helices will be discussed. This project is built though the collaboration and support from Dr. Faulon and the Sandia University Research Program.

CSRI POC: Mark D. (Danny) Rintoul III, (505) 844-9592

Title: Simulating High Speed Interconnects with the Georgia Tech Network Simulator

Speaker: George Riley, Georgia Tech

Date/Time: Wednesday, November 17, 2004, 9:00-10:00 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: The Georgia Tech Network Simulator (GTNetS) is a newly designed and implemented network simulation environment designed from the beginning for scalability and distributed execution. We will give a brief overview of the design and capabilities of this tool. Next we will present our ongoing work in using the GTNetS tool to model and predict the performance of Super-Computer Interconnect Networks. High Speed Interconnects are one of the important building blocks for building Super Computers and other High end computing platforms. Using GTNetS we are building a generic framework for evaluating various interconnect topologies and the associated switching and routing algorithms employed in building HPCs. Discrete Event simulation has long been used for evaluating network protocols in traditional IP based networks. Employing some of the network simulation principles in simulating high speed interconnects can provide a new approach to evaluating super computer architectures.

CSRI POC: Keith D. Underwood, (505) 284-9283

Title: Direct Rendering of Non-linear Objects

Speaker: Dr. Alyn Rockwood, Colorado School of Mines

Date/Time: Friday, June 11, 2004, 10:00-11:00 am (PDST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract: The classic computer graphics pipeline is fast and sophisticated, relying on piece-wise linear representations (polygonal facets) to attain efficiency. Unfortunately, the conversion of scientific data to polygon models often loses information through linearization and assumptions about topology. Particularly vulnerable to such loss are high frequency components that are often of primary interest.

Described is a point based, volume rendering method that makes no assumption about topology. Points are generated directly from the surface or volume in a fast forward scheme. These produce statistically accurate visualizations and can be used to focus on individual features such as iso-surfaces, and singular regions. Examples will be shown for high order finite elements and biomedical applications.

CSRI POC: Gary Templet, Jr., (925) 294-4540

Title: Uncertain Reasoning in Open Worlds

Speaker: Stuart Russell, Computer Science Division, University of California

Date/Time: Thursday, July 22, 2004, 10:00am - 11:00am (PDST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: There has been a good deal of progress in recent years on the problem of uncertain reasoning about objects and relations. With few exceptions, however, work in this area assumes *unique names* (every term in the modeling language refers to a distinct object) and *domain closure* (there are no objects besides those named by terms in the language). These assumptions are untenable in many real-world settings, where unknown objects may exist and there is uncertainty as to the true identity of objects. Such settings include surveillance, link detection, and information extraction. I will present a formal language for specifying probability models that allow for unknown objects and identity uncertainty, with applications to wide-area freeway traffic monitoring and bibliographic citation databases.

CSRI POC: Keith B. Vanderveen, (925) 294-3207
Monica Martinez-Canales, (925) 294-3157

Title: Multilevel Techniques for Quasilinear Partial Differential Equations

Speaker: Oliver Roehrle, University of Colorado

Date/Time: Thursday, March 18, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: The focus of this presentation is on efficient multilevel solvers for two-dimensional elliptic systems of nonlinear partial differential equations (PDEs), where the nonlinearity is of the type. The Navier-Stokes equations are an important representative of this class and are at the focus of this talk. Using a first-order system least squares (FOSLS) approach and introducing a new variable for, we obtain for this class of PDEs a formulation in which the nonlinearity appears as a product of two different variables. The result is a system that is linear within each variable but nonlinear in the cross terms. A nested Newton-FOSLS-Multigrid method strategy is developed and analyzed for solving this class of PDEs. A new projection multilevel (PML) method is also developed for handling the nonlinearity directly. Numerical as well as theoretical results are presented.

CSRI POC: Johnathan Hu, (925) 294-2931

Title: Studies of Time Integration Methods for Reaction-Diffusion Systems

Speaker: David Ropp, SNL

Date/Time: Thursday, March 25, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: In this first part of this talk we present numerical experiments of time integration methods applied to systems of reaction-diffusion equations. Our main interest is in evaluating the relative accuracy and asymptotic order of accuracy of the methods on problems, which exhibit an approximate balance between the competing component time scales. Such problems provide a challenging test for this evaluation and tend to reveal subtle differences between the various methods. The methods we consider include first- and second-order semi-implicit, fully implicit, and operator-splitting techniques. The test problems include a prototype propagating nonlinear reaction-diffusion wave, a non-quilibrium radiation-diffusion system, a Brusselator chemical dynamics system and a blow-up example. We find that while operator-splitting methods often obtain very good accuracy, they can also manifest a serious degradation in accuracy due to stability problems.

In the second part of the talk we further investigate the instabilities of second-order operator-splitting methods applied to the Brusselator equations. These instabilities are manifested as high wave number spatial errors. We present a theorem for stability of operator-splitting methods applied to linear reaction-diffusion equations with indefinite reaction terms, which controls both low and high wave number instabilities. However, if L-stable methods are used for the diffusion term the high wave number instability will be controlled more easily. In the absence of L-stability, an additional time step condition that suppresses the high wave number modes appears to guarantee convergence at the asymptotic order for the operator-splitting method. Numerical results for a model problem confirm this theory, and results for the Brusselator problem agree as well.

CSRI POC: David Womble, (505) 845-7471

Title: Post-Processing for Discontinuous Galerkin Methods

Speaker: Jennifer K. Ryan, Oak Ridge National Lab

Date/Time: Thursday, October 21, 2004, 9:30-10:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: In this talk, a brief introduction to the discontinuous Galerkin finite element method will be given along with a discussion of a post-processing technique for enhancing the accuracy of the method. The discontinuous Galerkin (DG) method is increasingly used in engineering applications because of its ability to handle complicated geometries, simple treatment of boundary conditions, high-order accuracy, flexibility for adaptivity, and because it is highly parallelizable. To fully utilize the potential of the inherent high order accuracy of the DG method, a post-processing technique is implemented. Typically, k+1 order accuracy is obtained using the discontinuous Galerkin method, where k is the highest degree polynomial used in the approximation. The post-processor allows improvement in accuracy for time-dependent linear hyperbolic equations from order k+1 to order 2k+1 when the equation is solved over a uniform mesh. A discussion of extending the results of the post-processor to include variable coefficient hyperbolic equations in one and two dimensions as well as one-sided post-processing and post-processing over a smoothly varying mesh will also be presented.

CSRI POC: Scott Collis, (505) 284-1123

Title: Learning Meaning via Unsupervised Development of Ontologies in Aid of Richer, more Precise and Complete Information Retrieval

Speaker: Joseph Saliba*, Sangita Ghosh*, Thomas Voth*, Eric Fowler*, Michael Rappaport*, Noel Jorden*, Alex Baia*, Matt Gadda*, Nate Repucci* and Alex Bäcker+
* University of Colorado at Boulder, + Sandia National Laboratories

Date/Time: Monday April 26, 2004 3:00-4:00 pm

Location: Building 980 Room 24 (Sandia NM)

Brief Abstract: We will introduce a prototype for a next-generation search engine that aims to a) deliver information, as opposed to web pages, in response to queries and b) understand the meaning of queries and results rather than look for words of one in the other.

When users of the World Wide Web perform a web search, they are usually looking for a piece of information or a particular file. Current generation search engines respond to queries with a list of URLs that link to web pages presumed to contain the information searched for. If a search engine's relevance ranking method is effective, a web page returned in response to a search will usually contain information relevant to the query. Given that the length of web pages can be substantial, though, a more precise indicator than the web page identifier (URL) would be useful. It's almost as if today's search engines are analogous to the "buses" of urban transport, leaving searchers at predefined stops (URLs), rather than taking them all the way to the desired information; we present an engine that will go the extra mile, a "taxicab" for the information age.

We will also introduce a system designed to automatically generate ontologies from web content via search engine technology. An ontology is a model of a particular field of knowledge - the concepts and their attributes, as well as the relationships between the concepts. Ontologies are useful for knowledge sharing and for all kinds of "intelligent" applications that "understand" the meaning of words. They are behind a new generation of information technologies.

Today's ontologies, however, are laboriously developed manually by human experts. This makes them hard to keep updated, and hard to transfer to new fields of knowledge. We will discuss our approach to this difficult problem of automatic ontology generation, present results, limitations, and discuss what the hard problems that we anticipate for the future are.

Finally, we will combine both systems, employing an automatically developed ontology to automatically expand web search queries to their semantic vicinity.

CSRI POC: Alex Backer, (505) 844-1100 and Danny Rintoul, (505) 844-9592

Title: Computational Systems Biology

Speaker: Herbert Sauro, Keck Institute , California Institute of Technology

Date/Time: Wednesday, March 3, 2004, 10:00-11:00 (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: One of the characteristics of computational systems biology is its reliance on a diverse range of interdisciplinary skills and knowledge. In this talk I will focus on two areas, the relevance of electrical engineering and control theory in systems biology and the importance of software requirements for systems biology. Although the emphasis in the recent past has been on the application of ideas and software from the computer science world, I feel that the one non-biological field that could contribute most to systems biology is electrical engineering. In terms of simulation capability, electrical engineers have considerable experience in simulating large systems; last but not least they have a deep understanding, both practically and theoretically, of how systems transmit and manipulate information, something which biological cells do every second of their lives.

CSRI POC: Elebeoba (Chi-Chi) May, (505) 844-9933

Title: Direct numerical simulation of a negatively buoyant jet in fluids with stable density stratification

Speaker: Samuel P. Schofield, University of Arizona

Date/Time: Monday, August 16, 2004, 10:30-11:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: The finite Reynolds number behavior of a negatively buoyant jet injected into a fluid with stable density stratification is examined. Three-dimensional and Hele-Shaw experiments have shown instabilities in the jet leading to varicose and sinusoidal modes. We utilize direct numerical simulation of the Boussinesq equations with high order spectral element methods to capture the instability modes and examine the roles of buoyancy, viscosity, salt advection, and diffusion.

CSRI POC: Mark A. Christon, (505) 844-8279

Title: Data-Intensive Applications on Heterogeneous Cluster Computers – The SplitStreams Approach

Speaker: Professor Karsten Schwan, Georgia Institute of Technology

Date/Time: Friday, June 18, 2004, 10:00-11:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Communication services are a key enabler for large-scale cluster applications. The SPLITS (Software architecture for Programmable, LIghtweighT Stream handling) permits applications to dynamically map to the underlying communication infrastructure those services that best suit their current needs. Going beyond `traditional' protocol-level functions like multicast or other collective communications, SPLITS permits remote graphics codes to map image cropping to a communication co-processor, thereby offloading the host's I/O infrastructure. SPLITS can also be used to `bridge' the operations of an attached graphics board with that of an attached network processor receiving incoming data, to eliminate the unnecessary use of host memory. More generally, SPLITS is used to map the operations performed by application-level overlays 'into' the communication infrastructure, to deal with machine or application heterogeneity, support XML-based operations, or perform data filtering or transcoding.

This talk presents the SPLITS communication architecture and its key communication abstraction, termed stream handlers. The purpose of SPLITS is to enhance the capabilities of cluster systems, by enabling developers to map service functionality into OS kernels and onto attached network processors (ANPs) so as to best use the combined ANP/host resources. Services are composed with stream handlers, and they run on ANPs, in the host kernel, or at application-level. SPLITS and stream handlers are implemented for hosts that run standard Linux OS kernels and for ANPs that are based on Intel's IXP network processor. Services realized with SPLITS include (1) the efficient processing of XML-structured data and (2) remote graphics and visualization actions that perform per-client customizations of visual displays. Experimental evaluations of SPLITS with NP/host combinations are shown to run more efficiently and offer improved service performance compared to those that use pure host-based implementations.

CSRI POC: Neil Pundit, (505) 845-7601
Rolf Riesen, (505) 845-7363

Title: Multiscale Methods in Science and Engineering

Speaker: Guglielmo Scovazzi, University of Texas at Austin

Date/Time: Wednesday, June 9, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)

Brief Abstract:

PART I: Hydro-SUPG, a new multiscale framework for Lagrangian Hydrodynamics

Lagrangian Hydrodynamics algorithms (or hydrocodes) were among the first algorithms in Computational Mechanics, as their early implementations date back to the Manhattan Project at Los Alamos. Hydrocodes are time-accurate algorithms for large-deformation transient analysis and have nowadays several applications: from weapon design/analysis in the defense industry to crash worthiness analysis in the car industry, from semiconductor design applications to computational Astrophysics. The current state of the art of such methods faces difficulties in attacking computations on unstructured triangular/tetrahedral meshes, of crucial importance to speed up the design process. A new approach based on a multiscale/SUPG stabilization, particularly well suited for such meshes will be presented and its potential will be assessed with numerical experiments. This concept has been developed in close cooperation with Sandia National Laboratories, Albuquerque (NM).

PART II: "Magic Carpets", a multiscale link between Continuous (CG) and Discontinuous Galerkin (DG) methods

One of the major drawbacks of the Discontinuous Galerkin method is its cost in terms of unknowns to be stored and computed, a serious constraint in its development and practical applicability. As an example, it is well known that on a three-dimensional tetrahedral mesh, with piecewise linear test/trial functions, the ratio between the DG/CG degrees-of-freedom per mesh node is 28, a very hard obstacle to overcome from the practical point of view. A completely new multiscale approach will be presented to address this issue, based on a splitting of the DG solution into a continuous part and discontinuous correction. By locally condensing the discontinuous correction in terms of the continuous part, the resulting method retains the advantages of a DG discretization at the cost of a CG implementation. Applications to scalar advection/diffusion problems will be presented and analyzed with numerical examples. This work has been developed in close cooperation with Sandia National Laboratories, Albuquerque (NM).

CSRI POC: Mark Christon, (505) 844-8279

Title: New Function Approximation Algorithms for Optimization of Nonconvex Complex Models With Application to Costly Functions Involving Partial Differential Equations

Speaker: Christine A. Shoemaker, Cornell University

Date/Time: Wednesday, March 24, 2004, 10:00-11:00 (PT)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: We present a strategy for the constrained global optimization of expensive black box functions using response surface models. A response surface model is simply a multivariate approximation of a continuous black box function which is used as a surrogate model for optimization in situations where function evaluations are computationally expensive.

Prior global optimization methods that utilize response surface models were limited to box-constrained problems, but one of our new methods (Regis and Shoemaker, Jn. Of Global Optimization, in press) can easily incorporate general nonlinear constraints. With this method, which we refer to as the CORS (Constrained Optimization using Response Surfaces) Method, the next point for costly function evaluation is chosen to be the one that minimizes the current response surface model subject to the given constraints and to additional constraints that the point be of some distance from previously evaluated points. The distance requirement is allowed to cycle, starting from a high value (global search) and ending with a low value (local search). The purpose of the constraint is to drive the method towards unexplored regions of the domain and to prevent the premature convergence of the method to some point that may not even be a local minimizer of the black box function. The new method can be shown to converge to the global minimizer of any continuous function on a compact set regardless of the response surface model that is used.

Numerical results will be shown for our two response surface algorithms on a range of problems including test functions for global optimization and some complex real environmental problems based on field data that require as long as 3 hours per simulation. The response surface method performs very well in comparison to other optimization methods.

I will also discuss the development of a new parallel algorithm MAPO that utilizes function approximation methods. Numerical results will be presented that demonstrates that MAPO is more robust and faster than other alternatives.

Joint work with Prof. Shoemaker's Ph.D. student Rommel Regis, Operations Research and Industrial Engineering

CSRI POC: Patty Hough, (925) 294-1518

Title: ChaMPIon/Pro: High Performance MPI-2 for Scalable Parallel Computers and File Systems

Speaker: Anthony Skjellum and Rossen Dimitrov, Verari Systems, Inc.
(formerly Racksaver, Inc. and MPI Software Technology, Inc.)

Date/Time: Friday, May 7, 2004, 10:00-11:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: In this talk, we discuss the experiences with the full deployment of ChaMPIon/Pro for ASCI-scale clusters and other parallel systems including the Dell Tungsten Cluster at NCSA. Experiences with the standard, support Myrinet + TCP/IP at massive scale, and fully conforming to the MPI-2.1 standard are covered. Issues with interactions of file systems, including Lustre and others are mentioned. Benefits of thread-safe MPI based on the "fastest time to solution metric" instead of "minimum latency" metric are covered. Conclusions drawn in the MPI Software Pathforward project on tri-lab systems are mentioned as well.

CSRI POC: Ron Brightwell, (505) 844-2099

Title: Cray MTA-2 and Eldorado: Parallel Computing Made Easier

Speaker: Burton Smith & Simon Kahan, Cray, Inc.

Date/Time: Friday, October 22, 2004, 9:00-10:30 am (MT)

Location: Building 980 Room 95 (Sandia NM)
Building 915/W133 (Sandia CA)

Brief Abstract: The Cray MTA-2 is a multithreaded computer system that enables straightforward parallel programming and predictable performance. We provide the motivation for multithreading itself, followed by a quick introduction to the features of the MTA-2 and to Cray's plans for multithreading, including an overview of Eldorado: a multithreaded Red Storm.

We follow the introduction with some specific examples illustrating programming ease, predictability, and the domain of applicability.

CSRI POC: Bruce Hendrickson, (505) 845-7599

Title: Iterative validation: a scheme for improving the reliability and performance of eigenvalue block iterative solvers

Speaker: Andreas Stathopoulos and James R. McCombs, College of William and Mary

Date/Time: Monday, April 26, 2004, 10:00-11:00 am

Location: Building 980 Room 24

Brief Abstract: Krylov and Krylov-like iterative methods are the only means of obtaining a few extreme eigenpairs of huge, sparse, symmetric matrices. However, when the matrix cannot be factored, we cannot guarantee that no eigenvalues are skipped. The situation is worse with poorly separated (clustered) eigenvalues, while in theory exact multiplicities are guaranteed to be skipped in theory.

To improve robustness of eigensolvers in such cases, block Krylov methods are often used that work on multiple vectors at a time and thus can identify all clustered or multiple eigenvalues within the size of the block. Yet, eigenvalues can still be missed beyond the block size. Further, computational and numerical trade-offs make the choice of block size difficult.

Alternatively, a large number of eigenvalues can be obtained through a stable form of deflation called locking. When an eigenvalue λ converges, all subsequent computations are performed orthogonally to the corresponding eigenvector x. In practice, locking does not often miss eigenvalues and by relying on numerical noise it even identifies multiplicities for low tolerances. Yet, block methods are more effective with high multiplicities.

We propose a new technique, which we call {\it iterative validation of eigensolvers (IVE)}, that acts as a wrapper calling another eigenvalue block iterative method repeatedly until no missed eigenvalues can be identified. The inner method can be any block iterative method, such as block Lanczos or subspace iteration, that implements locking against an externally provided set of vectors.

IVE is a relatively unobtrusive way to validate results, dramatically improving robustness hence justifying the additional expense. Moreover, it provides a dynamic way to fine tune the block size without wasting all previous effort. Finally, assuming a multiplicity or a cluster of m eigenvalues, a block size of m would be slower for many required eigenvalues that do not belong to the cluster or the multiplicity. Iterative validation with an original block size of 1 finds first the easier part of the spectrum and it only uses the block size m at the clusters that need it. We discuss our implementation and prove its concept through several Matlab experiments with irbleigs and a block Jacobi-Davidson.

CSRI POC: Rich Lehoucq, (505) 845-8929

Title: A Meta-Partitioner for Faster Supercomputer Simulations

Speaker: Johan Steensland, Sandia National Laboratories, Livermore, California

Date/Time: Tuesday, November 23, 2004, 9:30-10:30 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: Structured adaptive mesh refinement (SAMR) methods are being widely used for computer simulations of various physical phenomena. Parallel implementations potentially offer realistic simulations of complex, three-dimensional applications. But achieving good scalability for large-scale applications is non-trivial. Performance is limited by the partitioner's ability to efficiently use the underlying computer's resources. The goal of our research project is to improve scalability for general SAMR applications executing on general parallel computers. We engineer the dynamically adaptive meta-partitioner, able to select and configure the most appropriate partitioning method at run-time, based on system and application state. This presentation gives an overview of our project, reports on recent achievements, and discusses the project's significance in a wider scientific context.

CSRI POC: Karen Devine, (505) 845-7585

Title: Multigrid with Cache Optimizations on Adaptive Mesh Refinement Hierarchies

Speaker: Danny Thorne, Florida International University

Date/Time: Wednesday, March 17, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: Patch-based adaptive mesh refinement has become an attractive technique for spatial discretization in a host of scientific simulations, ranging from shock hydrodynamics to combustion and plasma physics. The ability to place a refined patch (with a Cartesian mesh) at any arbitrary location in the domain obviates the need for mesh stretching and promotes its use with higher-order stencils. Conformal transformation techniques have extended this technique to nonrectangular/cuboid domains of sufficient complexity to meet the needs of scientific (as opposed to engineering) simulations. A large number of scientific problems (e.g., combustion, incompressible hydrodynamics, magnetohydrodynamics, etc.) frequently pose a Poisson problem with variable coefficients as a part of their solution strategy. While this could be formulated as a giant A x = b problem and treated with iterative methods (e.g., Krylov methods), the multilevel nature of the grid strongly suggests multigrid approaches. Further, the (relatively) small data set associated with a patch lends this approach to cache-based optimization of numerical operations local to a patch, i.e., smoothing. In this work, we use a combination of adaptive refinement and multilevel procedures to solve variable coefficient elliptic boundary value problems. This research focuses on (a) implementing cache aware optimizations to multigrid in an AMR context and (b) modifying the AMR multigrid algorithm to do only post-smoothing so that the cache aware optimizations will have a greater effect. Cache aware algorithms are designed to minimize the number of times data goes through cache, thereby increasing the efficiency of the algorithm. Cache memories are much faster than main memory, so the CPU can be kept more busy when it is getting data from cache memories. In an AMR context, we modify Gauss-Seidel so that all the data required by the smoothing iterations needs to be brought into a cache only once, not many times, and it still gets the exact same answer as the standard algorithm (i.e., bitwise compatibility). In order to further improve the efficiency of cache usage, we do only post-smoothing and combine the residual computation with the smoother. In this way all of the smoothing and the residual computation for each level of a V cycle can be accomplished while bringing the data into cache just once (ideally). Doing post-smoothing only is a substantial change in the AMR algorithm. It is

especially useful when implementing cache aware algorithms. We see better cache effects when more smoothing iterations are done consecutively. Further, reducing the work that is done outside of the smoother means that speeding up the smoother will have a greater impact on the whole algorithm.

CSRI POC: Jonathan Hu, (925) 294-2931

Title: Bridging Between QM and Mesoscale: Development and Application of ReaxFF Reactive Potentials for Metal and Metal Oxide Surface Catalysis

Speaker: Adri van Duin, Caltech Materials and Process Simulations Center

Date/Time: Monday, November 15, 2004, 2:00 - 3:00 pm

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: The high computational expense of quantum chemical (QM) methods greatly hinders application of these methods to dynamic simulations of the interaction of metal and metal oxide surfaces with their catalytic substrates. As such, application of QM methods tends to be limited to idealized, static simulations. While such simulations have provided valuable insights in metal and metal oxide surface catalysis, they cannot provide a full picture of the chemical complexity and the influence of reaction conditions (temperature, pressure, chemical composition) on the catalytic process.

To provide a dynamic picture of chemical reactivity at metal/metal oxide surfaces for large (>1000 atoms) systems we have extended the ReaxFF reactive potentials1-4 to various metal and metal oxides and their interaction with first-row elements. We have fitted ReaxFF parameters to extensive QM-databases covering both ground state systems and relevant reaction pathways. Using this method we have performed dynamical simulations of oxygen, hydrogen and hydrocarbon interactions with metal and metal oxide systems and have managed to abstract reaction kinetic data from these simulations that can be used to train mesoscale fuel cell models.

1: A.C.T. van Duin, S. Dasgupta, F. Lorant and W.A. Goddard (2001) J. Phys. Chem. A 105, 9396-9409.
2: A. Strachan, A.C.T. van Duin, D. Chakraborty, S. Dasgupta and W.A. Goddard (2003) Phys. Rev. Letters 91, 098301-1.
3: A.C.T. van Duin, A. Strachan, S. Stewman, Q. Zhang, X. Xu and W.A. Goddard (2003), J. Phys. Chem. A 107, 3803-3811.
4: Q. Zhang, T. Cagin, A.C.T. van Duin, W.A.Goddard, Y. Qi and L.G. Hector (2004) Phys. Rev. B 69, 045423.

CSRI POC: Richard Muller, (505) 284-3669

Title: Chemical Reactions and Excitons in Amorphous Silica

Speaker: Renee van Ginhoven - Post Doc Seminar, Commissariat a L'Energie Atomique (CEA) Saclay, France

Date/Time: Tuesday, April 27, 2004, 9:00-10:00 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: The reaction of water with amorphous silica networks and self-trapping of triplet state excitons were investigated using density functional theory (DFT) with periodic boundary conditions. It has been well established that the simulation of amorphous networks requires large systems. Since the system size accessible to DFT is on the order of 100 atoms, the statistics for the short and medium range structure were improved by the use of multiple samples. Reactivity and exciton localization are shown to be correlated with both local structure and network relaxation. The use of multiple small systems is shown to be a useful approach for the study of processes in glass that require the use of electronic structure methods.

The study of diffusion of helium in silicon carbide will also be discussed.

CSRI POC: John Aidun, (505) 844.1209

Title: Approximation and Optimal Control of a Convection-Diffusion System

Speaker: Eric Vugri, Virginia Polytechnical Institute

Date/Time: Tuesday, February 10, 2004, 9:00-10:00 am (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: "Traditionally, eigenvalue analysis has been used to predict the long-term behavior of physical systems. However, eigenvalue analysis has been shown to be insufficient when studying the linear stability of many systems occurring in fluid dynamics. Recently, the normality of systems has been used to study and explain the transient and asymptotic behavior. Additionally, when utilizing techniques from optimal control, the normality of a system can have additional significant impacts.

In this talk, we briefly review basic concepts from optimal feedback control, and how the normality of a system can impact approximation of these systems. For an optimal control problem governed by a convection-diffusion system, we examine three different approximation schemes and how the different approximation techniques impact computation of eigenvalues, feedback gains, and numerical solutions to algebraic Riccatti equations."

CSRI POC: David Womble, (505) 845-7471

Title: Coupling of Atomistic and Continuum Simulations using a Bridging Scale Decomposition

Speaker: Greg Wagner, SNL, Livermore, CA

Date/Time: Monday, January 19, 2004, 9:00-10:00 am

Location: Building 980 Room 95

Brief Abstract: Molecular dynamics (MD) simulations have become a prominent tool for elucidating complex physical phenomena in solid mechanics, such as fracture, surface friction, and plasticity. However, the length and time scales that can be probed using MD are limited by computational cost to nanoseconds and tens of nanometers, suggesting that more creative techniques must be used to study longer-ranged effects. In this talk, a new method for coupling MD and continuum mechanics simulations is presented that is based on the projection of the MD solution onto coarse scale shape functions. This projection, or "bridging scale", represents that part of the solution that is obtainable by both the MD and continuum solution methods. By subtracting the bridging scale from the total solution, we obtain a coarse-fine decomposition that decouples the kinetic energy of the two simulations. The resulting decomposition can be used in a dynamic, finite-temperature simulation method in which MD is used only in a localized region, while the continuum simulation covers the entire domain, including the MD region to which it is coupled. The proper boundary condition for the MD region can be derived by eliminating analytically the fine scale degrees of freedom that are not represented by the coarse scale; it is demonstrated through several simple examples that this boundary condition gives the correct transfer of energy out of the MD region. Progress is shown in applying the method to applications including crack propagation and nanoindentation.

CSRI POC: Scott Collis, (505) 284-1123

Title: Identifying Monitoring Locations in a Water Distribution System Using Simulation and GIS

Speaker: Thomas M. Walski, Haestad Methods, Inc

Date/Time: Friday, December 17, 2004, 10:00–11:00 am

Location: Building 980, Room 95 (Sandia NM)

Brief Abstract: Selecting the best sites to locate water quality and pressure monitoring locations involves satisfying multiple objectives and involves using a good deal of judgment. This paper looks at using the results of a water distribution model combined with the capability of spreadsheet calculations, GIS and the water distribution model for decision support. The approach used involves calculating indexes describing the desirability of sites for monitoring locations based primarily on ease of access and variation in the attribute of water age and pressure.

CSRI POC: Jon Berry, (505) 284-4021

Title: Comparing Optimization Methods for the Temperature Inversion problem

Speaker: Professor Darrell Whitley, Colorado State University

Date/Time: Friday, April 2, 2004, 11:00-12:00 noon (MST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 108 (Sandia CA)--videoconference

Brief Abstract: Several inverse problems exist in the atmospheric sciences that are computationally costly when using traditional gradient-based methods. One such problem is to infer temperature profiles based on radiance observations. The goal is to compute these inverses in real-time: in this case, the inverse much be computed 8 times a second to match the kilometer per-second speed of the earth observing satellites collecting the radiance data. This would seem to be a good application for heuristic search methods. Unfortunately, commonly used heuristic search methods, including local search and various evolutionary algorithms, do not perform well on these problems. This research investigates why the temperature inversion problem is difficult and what this implies for various search methods. One cause of difficulty is the occurrence of curved ridges in the evaluation space. Two solutions to this problem are explored: the use of rotated representations using Principal Component Analysis and the use of smoothness constraints. Constraint-based search methods prove to be much more efficient and effective than other search methods for temperature inversion.

CSRI POC: Jean-Paul Watson, (505) 845-8887

Title: Primal constraints for FETI-DP and Neumann-Neumann Algorithms for three-dimensional Linear Elasticity

Speaker: Olof B. Widlund, Courant Institute of Mathematical Sciences

Date/Time: Monday, July 8, 2004, 11:30-12:30 am (MDST)

Location: Building 980 Room 24 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: The FETI and Balancing Neumann-Neumann algorithms form two of the three families of domain decomposition methods that have been most carefully implemented and severely tested on the very largest existing parallel computer systems; the third is the family of Overlapping Schwarz methods with at least two levels.

In many ways, the design of the coarse second level of the preconditioners is central. It is important to keep it small since all other components of the preconditioners parallelizes across the processors of a parallel or distributed computer. We note that a second level is necessary in order to make the computation scalable for elliptic problems, i.e., to obtain a convergence rate of the iteration, which is independent of the number of local problems.

We will only discuss problems in three dimensions. For the classical Balancing Neumann-Neumann algorithm, the global space has a dimension of six times the number of floating substructures; it also helps to include six degrees of freedom for the substructures that are constrained by boundary conditions. This count is a direct reflection of the fact that there are six linearly independent rigid body modes;
The same count is also typical for the coarse space of standard Overlapping Schwarz methods, which include a second coarse level.

The analysis of the FETI methods has posed a very real challenge but by now a coherent theory has emerged. Algorithmically and theoretically, the main research focus is now on the Dual-Primal FETI methods. Previous theoretical work on scalar elliptic problems, such as those arising in heat conduction in highly heterogeneous materials, has recently been extended to linear compressible elastic materials obtaining convergence rates of the iteration which are independent of even large changes in the Lam\'{e}parameters across the interface between the subdomains. We note that there are also interesting problems of numerical linear algebra related to these algorithms.

CSRI POC: Kendall H. Pierson, (505) 284-5894

Title: Introduction to Domain Decomposition

Speaker: Olof B. Widlund, Courant Institute of Mathematical Sciences

Date/Time: Monday, July 12, 2004, 9:00-10:00 am (MDST)

Location: Building 980 Room 95 (Sandia NM)
Building 921 Room 137 (Sandia CA)--videoconference

Brief Abstract: Two main families of domain decomposition methods are introduced in a framework of finite elements. All these methods provide preconditioners for conjugate gradient and other Krylov space algorithms and they are all built from components involving the exact or approximate solution of the given problem restricted to many subregions into which the original domain has been partitioned. In addition, a coarse component is also required in order to ensure scalability, i.e., a convergence rate of the iteration, which is independent of the number of subproblems. The coarse problem will typically involve a few degrees of freedom per subdomain.

Of the two families, the Iterative Substructuring Methods are based on a decomposition of the region into nonoverlapping subdomains and an interface. In a successful iteration, the values of the degrees of freedom on the interface are obtained quickly and those interior to the subdomains are then obtained in a local computation on the individual subdomains. Examples of successful methods of this type will be given as well as an overview of current knowledge, in particular, concerning the type of continuum mechanics problems for which they can be used reliably.

The Overlapping Schwarz Methods, on the other hand, are based on a partitioning of the region into overlapping subdomains and the rate of convergence will depend on the relative overlap of neighboring subdomains and the quality of the coarse, global component of the preconditioner. These methods have been used extensively in many applications and an overview will be given of the present theory.

CSRI POC: Kendall H. Pierson, (505) 284-5894

Title: Model Order Reduction for Large-Scale Applications

Speaker: Karen Willcox, Massachusetts Institute of Technology

Date/Time: Thursday, August 26, 2004, 9:30-10:30 am

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: Model reduction is a powerful tool that allows the systematic generation of cost-efficient representations of large-scale systems resulting from discretization of PDEs. Reduction methodology has been developed and applied for many different disciplines, including controls, fluid dynamics, structural dynamics, and circuit design. This seminar will discuss model reduction of computational fluid dynamic (CFD) systems, although the techniques presented are applicable to general systems of PDEs. Examples will be given from a range of unsteady flow applications, including flow sensing and reconstruction, active flow control, and compressor blade aeroelasticity.

CSRI POC: Bart van Bloemen Waanders, (505) 284-6746

Title: Connecting MRP, MRP II and ERP Supply Chain Planning via Optimization Models

Speaker: David L. Woodruff, University of California, Davis

Date/Time: Thursday, August 12, 2004, 3:00-4:00 pm

Location: Building 980 Room 95 (Sandia NM)

Brief Abstract: We focus on optimization applications in production planning in a supply chain. We demonstrate by construction that we can begin with MRP and MRP II and end up with a useful basis for a planning model. In order to produce a useful model, we add extensions and ultimately arrive at models that bear little resemblance to MRP and certainly solutions for the optimization problems cannot be obtained using MRP or MRP II processing or logic. As time permits, we will highlight connections with hierarchical systems for planning and detailed scheduling.

CSRI POC: Jean-Paul Watson, (505) 845-8887

Chapter 6. Fellowships

The Computer Science Research Institute supported two students during CY2004 through the DOE High Performance Computer Science (HPCS) Fellowship administered by the Krell Institute. The objective of the DOE High-Performance Computer Science Fellowship program is to encourage the training of computer scientists by providing financial support to talented students to enter a period of study and research in computer science with an emphasis on high-performance computing, accompanied by practical work experience with researchers at Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and Sandia National Laboratories.

The fellowship program requires a program of study that will provide a solid background in high-performance computing. Examples of research specializations of interest to the program include:

- Parallel and novel architectures, including clusters of SMPs
- Three-dimensional scientific visualization
- High-speed network interconnects
- Parallelizing compiler technology
- Parallel systems software (OS kernel technology, file systems, etc.)
- Performance evaluation and modeling
- Scalable computer security
- Object-oriented scientific programming frameworks
- High-performance computing software component frameworks
- Parallel scalable algorithms

After the start of the fellowship, each participant will participate in a research assignment (practicum) at Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), or Sandia National Laboratories (SNL) working with high-performance computing researchers. During the summer of 2004, Anne Shepherd, an HPCS fellow studying at the College of William and Mary completed her practicum at Sandia National Laboratories working with CSRI researcher Bill Hart.

Students must be United States citizens planning full-time, uninterrupted study toward a Ph.D. degree at a U.S. university. Students who are senior undergraduates or in their first or second year of graduate study in computer science are eligible to apply for the DOE High-Performance Computer Science Graduate Fellowship (DOE HPCSF).

For additional information regarding the Krell Institute and the HPCS fellowship, please see the web site http://www.krellinst.org.

Chapter 7. For More Information

For more information about the CSRI, please contact one of the following:

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Appendix A. Distribution:

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