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ISCR FY2005 Annual Report

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February 7, 2006

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ISCR

Institute for Scientific Computing Research

Annual Report

Fiscal Year 2005

Lawrence Livermore National Laboratory,
P.O. Box 808, L-419, Livermore, CA 94551

UNIVERSITY RELATIONS PROGRAM

The University Relations Program (URP) encourages collaborative research between Lawrence Livermore National Laboratory (LLNL) and the University of California campuses. The Institute for Scientific Computing Research (ISCR) actively participates in such collaborative research, and this report details the Fiscal Year 2005 projects jointly served by URP and ISCR. For a full discussion of all URP projects in FY 2005, please request a copy of the URP FY 2005 Annual Report by contacting:

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Director's Report

Large-scale scientific computation and all of the disciplines that support and help validate it have been placed at the focus of Lawrence Livermore National Laboratory (LLNL) by the Advanced Simulation and Computing (ASC) program of the National Nuclear Security Administration (NNSA) and the Scientific Discovery through Advanced Computing (SciDAC) initiative of the Office of Science of the Department of Energy (DOE). The maturation of simulation as a fundamental tool of scientific and engineering research is underscored in the President's Information Technology Advisory Committee (PITAC) June 2005 finding that "computational science has become critical to scientific leadership, economic competitiveness, and national security."

LLNL operates several of the world's most powerful computers—including today's single most powerful—and has undertaken some of the largest and most compute-intensive simulations ever performed, most notably the molecular dynamics simulation that sustained more than 100 Teraflop/s and won the 2005 Gordon Bell Prize.

Ultrascale simulation has been identified as one of the highest priorities in DOE's facilities planning for the next two decades. However, computers at architectural extremes are notoriously difficult to use in an efficient manner. Furthermore, each successful terascale simulation only points out the need for much better ways of interacting with the resulting avalanche of data. Advances in scientific computing research have, therefore, never been more vital to the core missions of LLNL than at present.

Computational science is evolving so rapidly along every one of its research fronts that to remain on the leading edge, LLNL must engage researchers at many academic centers of excellence. In FY 2005, the Institute for Scientific Computing Research (ISCR) served as one of LLNL's main bridges to the academic community with a program of collaborative subcontracts, visiting faculty, student internships, workshops, and an active seminar series.

The ISCR identifies researchers from the academic community for computer science and computational science collaborations with LLNL and hosts them for both brief and extended visits with the aim of encouraging long-term academic research agendas that address LLNL research priorities. Through these collaborations, ideas and software flow in both directions, and LLNL cultivates its future workforce. The Institute strives to be LLNL's "eyes and ears" in the computer and information sciences, keeping the Laboratory aware of and connected to important external advances. It also attempts to be the "hands and feet" that carry those advances into the Laboratory and incorporate them into practice.

ISCR research participants are integrated into LLNL's Computing Applications and Research (CAR) Department, especially into its Center for

Applied Scientific Computing (CASC). In turn, these organizations address computational challenges arising throughout the rest of the Laboratory. Administratively, the ISCR flourishes under LLNL's University Relations Program (URP). Together with the other four institutes of the URP, the ISCR navigates a course that allows LLNL to benefit from academic exchanges while preserving national security. While it is difficult to operate an academic-like research enterprise within the context of a national security laboratory, the results declare the challenges well met and worth the continued effort.

FY 2005 was the sixth full year under Acting Director David Keyes. The Fu Foundation Professor of Applied Mathematics at Columbia University and an ISCR faculty participant since October 1997, Keyes dedicated one-third of his time to the technical program of the ISCR. James McGraw continued as the Deputy Director of the ISCR with Linda Becker as the Institute Administrator. Paula Ashley, Erica Dannenberg, Pamela Mears, Lisa Nobida, and Tiffany Ashworth logistically supported the large visitor and summer programs of the ISCR.

The ISCR continues to have a small contingent of research staff members within its organization, including Nelson Max, Garry Rodrigue, and Rao Vemuri, who all hold joint appointments as professors at UC Davis and senior researchers at LLNL. In addition, the ISCR hosted 10 graduate students (listed in Table 1), including 6 who hold Student-Employee Graduate Fellowships (SEGRF) through LLNL's URP. This fellowship program enables students to work part time with LLNL researchers while pursuing their Ph.Ds. The remaining four graduate students are here on independent co-op programs.

The ISCR enables substantial interactions between academia and LLNL staff via consultants and participating guests. Consulting agreements are vehicles for permitting academics to interact with LLNL in a compensated fashion. Consultants may serve on review committees, present short courses,

Table 1. Students on a Student-Employee Graduate Fellowship (SEGRF) or other LLNL-sponsored fellowship.

Student	University	LLNL Advisor(s)
Janine Bennett	UC Davis	Valerio Pascucci
Sam Brockington	UC Davis	Garry Rodrigue & Dave Hwang
Paul Castellucci	Stanford University	Rose McCallen
Aaron Fisher	UC Davis	Garry Rodrigue
Aaron Herrnstein	UC Davis	Michael Wickett
Michael McConnehey	UC Davis	Garry Rodrigue
Andrew Nonaka	UC Davis	David Trebotich
Joshua Senecal	UC Davis	Mark Duchaineau
Krell Tengesdal	UC Davis	Garry Rodrigue
Sage Weil	UC Santa Cruz	Tyce McLarty

Table 2. The 12 ISCR consultants for FY 2005.

Consultant	Affiliation	LLNL Contact
Randolph Bank	UC San Diego	Rob Falgout
Achiezer Brandt	UCLA	Rob Falgout
Marsha Berger	New York University	Andy Wissink
Anne Greenbaum	University of Washington	Peter Brown
Charles Hansen	University of Utah	Mark Duchaineau
Heinz-Otto Kreiss	UCLA	Lori Diachin & Bill Henshaw
Thomas Manteuffel	CU-Boulder	Rob Falgout & Peter Brown
Stephen McCormick	CU-Boulder	Rob Falgout & Peter Brown
Gregory Miller	UC Davis	David Trebotich
Linda Petzold	UC Santa Barbara	Carol Woodward & Radu Serban
David Saloner	University of San Francisco	David Trebotich
Homer Walker	Worcester Polytechnic Institute	Peter Brown

and visit LLNL periodically for technical meetings. All consultants have a specific LLNL technical point of contact for overseeing their interactions. Table 2 lists the 12 ISCR consultants for FY 2005.

Participating guests are researchers from academia or industry that often need intermittent access to LLNL staff and facilities. This status permits an appropriate security clearance and the ability to quickly arrange for onsite visits with LLNL staff over a period of time ranging from one month to two years. Table 3 lists ISCR's 36 participating guests for FY 2005.

The pages of this annual report summarize the activities of the faculty members, postdoctoral researchers, students, and guests from industry and other laboratories who participated in LLNL's computational mission under the auspices of the ISCR during FY 2005. These activities, which are further detailed in the accompanying CD-ROM and Web site, fall under two main themes: sponsored-

Table 3.
ISCR's 36 participating guests for FY 2005.

Guest	Affiliation	LLNL Contact
Gregory D. Benson	University of San Francisco	Patrick Miller
Peer-Timo Bremer	UC Davis	Valerio Pascucci
Marian Brezina	CU-Denver	Rob Falgout
Zhiqiang Cai	Purdue University	Barry Lee
Alok Choudhary	Northwestern University	Terence Critchlow
Jennifer Dacles-Mariani	UC Davis	Garry Rodrigue
Hans de Sterck	CU-Boulder	Rob Falgout
Branden E. Fitelson	UC Berkeley	Terence Critchlow
Franz Franchetti	Carnegie Mellon University	Kim Yates
Alejandro Garcia	San Jose State University	James McGraw
Izaskun Garrido-Hernandez	University of Bergen, Norway	Van Emden Henson
Charles W. Gear	Princeton University	Steve Lee
Jerrold R. Goodwin	University of San Francisco	Pete Wells
Bernd Hamann	UC Davis	Mark Duchaineau
Alan Hindmarsh	LLNL Retiree	Carol Woodward
Martin Isenburg	University of North Carolina	Bronis de Supinski
Kenneth I. Joy	UC Davis	Mark Duchaineau
Johannes Kraus	University of Loeben	Van Emden Henson
Ramya Krishnamurthy	Oak Ridge National Laboratory	Terence Critchlow
Oren Livne	University of Utah	Van Emden Henson
Bertram Ludaescher	San Diego Supercomputer Center	Terence Critchlow
Jeanne T. Martin	LLNL Retiree	Bronis de Supinski
Stephen F. McCormick	CU-Boulder	Rob Falgout
Sally McKee	Cornell University	Bronis de Supinski
Frank R. Mueller	North Carolina State University	Bronis de Supinski
Harry L. Nelson	LLNL Retiree	Bronis de Supinski
Mary Elizabeth Ong	Former LLNL Employee	Van Emden Henson
Peter S. Pacheco	University of San Francisco	Patrick Miller
Markus Pueschel	Carnegie Mellon University	Kim Yates
Subhash Saini	NASA Ames Research Center	Don Dossa
Paul E. Saylor	University of Illinois	Steven Lee
Keith Seymour	University of Tennesee	Dan Quinlan
Claudio Silva	University of Utah	Daniel Laney
Lansing Sloan	LLNL Retiree	Pete Eltgroth
Gabriel Wittum	Universität Heidelberg	Rob Falgout
Haihang You	University of Tennesee	Dan Quinlan

research activities that stimulate interactions between academia and LLNL staff, and a diverse visitor program that enables both short- and long-term residential stays at LLNL.

ISCR oversees three different types of sponsored-research activities. The University Collaborative Research Program (UCRP), through the ISCR, funded seven research projects during FY 2005 at University of California campuses that supported graduate students working on doctoral thesis research. Along with their respective faculty principal investigators, the students worked closely with an LLNL collaborator.

The ISCR also coordinated the funding of 24 research subcontracts to various academic institutions throughout the United States. These contracts are normally funded by programs at LLNL to help address long-term Laboratory requirements and are used to fund sabbatical visits to LLNL for three to six months. Eleven faculty members spent at least a portion of their sabbatical leave here during FY 2005.

With Laboratory Directed Research and Development (LDRD) funds, the ISCR also supports Exploratory Research in the Institutes (ERI), which awards research grants to LLNL staff with the goal of developing ties to academia through co-funded research projects. The ISCR oversaw three such projects in FY 2005. Annual summaries for LDRD projects, UCRP projects, and subcontracts can be found in the next three sections of this document.

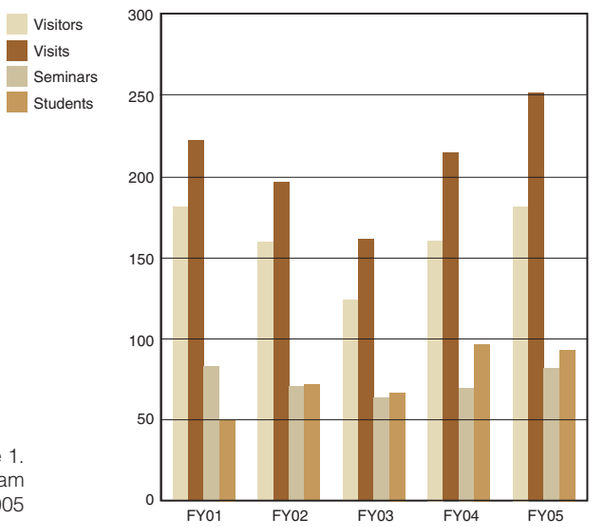

Figure 1.
ISCR Visitor Program
FY2001–FY2005

In FY 2005, the ISCR continued its tradition of maintaining an extensive and diverse Visitor Program, which includes sabbatical visitors, sponsored workshops, summer students, and various seminars featuring external speakers. Altogether, the ISCR hosted 252 visits from 182 different visitors, an average of more than four visits per week. The vast majority of the visitors (72%) were from academia, with 11% from industry, 10% from other federal laboratories, and 7% from non-laboratory-based government institutions. Visitors from outside the United States made up 22% of the total.

The ASC Institute for Terascale Simulation Lecture Series was established in 2000 to enrich the intellectual atmosphere of LLNL's large simulation community through the visits of leaders representing the diverse areas of computation. In FY 2005, we hosted five speakers in this series. The general ISCR seminar series included an additional 76 talks covering a wide spectrum of research areas. Titles of these talks can be found in the Seminar Series section of this report, and associated abstracts are linked on the accompanying CD-ROM and Web site.

During the summer, ISCR hosted 91 visiting students for a total student population during the summer of 101 (counting the students in Table 1 in residence year round). The summer program exposes students to the stimulating and challenging work environment of a national laboratory. Successful candidates are hired as summer employees, assigned individual LLNL mentors, and given specific projects to which they will contribute. The nature of the project is appropriate to the student's background and skills, and ranges from programming tasks to original research.

The topical coverage of the summer research program broadens each year as computation expands into new scientific areas and as computational tools become more powerful and diverse. Scalable algorithms, radiation transport, genomics, terascale visualization, and computer security are just a handful of topics from last summer's lively hallway conversations at the ISCR. The summer program runs from May to September, with most participants

spending 10–12 weeks on site. Project reports for most of the students can be found on the accompanying CD-ROM and Web site.

In June, with the advent of our large student summer program, we ramped up our sixth annual Summer Student Lecture Series. The lectures fell into one of two categories—Computational Modeling at the Terascale and Computer Science at the Terascale—and were intended for students, but permanent CASC researchers also attended. The 19 lecturers are listed in the Seminar Series section of this annual report, and full summaries are available on the accompanying CD-ROM and Web site.

Poster presentations were made by 65 ISCR summer students at the LLNL Student Research Symposium in August 2005. The event, held at LLNL's Central Café, attracted local media and scientific staff from across the Laboratory, as well as other students and summer research mentors. Overall, 155 students presented posters, making ISCR's share about 42% of the total. Poster topics covered diverse topics from performance-modeling tools to management of data in petabyte-scale file systems, and participants ranged in seniority from first-year, community-college students to graduate students about to complete their doctorates.

Figure 1 charts the numbers of visitors and seminars over the past five years. The number of students in residence in FY 2004 increased substantially due to the expansion of the ISCR's responsibility in LLNL's summer programs and decreased slightly in FY 2005 due to an across-the-board reduction in educational program funds from central NNSA Headquarters.

LLNL organizations, who have come to depend on the burst of effort summer students can lend to their programs, made up part of the reduced contribution from Washington, and CASC scientists mentored 61% of these students. Other LLNL organizations mentoring ISCR summer students were: AX Division, Center for Applications Development and Software Engineering (CADSE), DNT & PAT Computing Applications Division (DCOM), Energy, Environment, and Biology (EEBI), Environmental Protection Division (EPD), Integrated Computing and Communications Department (ICCD), NAI Computing (NAIC), and NIF and Engineering (NIFE). Some of these students elected to spend internships prescribed by their national fellowships at the ISCR, at no direct cost to LLNL, including DOE Computational Science Graduate Fellowship (CSGF) holders and Department of Homeland Security fellows.

Finally, the ISCR sponsored or co-sponsored eight off-site scientific workshops in FY 2005 in cooperation with other organizations. In each case, there was a vital LLNL interest and typically, several Laboratory researchers participated. In addition to the scientific workshops, ISCR also sponsored the UCLA Institute for Pure and Applied Mathematics (IPAM) Research in Industrial Projects for Students (RIPS) program. These sponsorships are listed later in this report and online reports are linked.

Most of the raw material of this document comes directly from the visitors and principal investigators of the projects being reported. We thank Arnold Gatilao for his editorial work and Alex Ballard of LLNL's Technical Information Department for her graphic artistry in producing an easily navigable and visually pleasing document.

We hope that you enjoy examining this report on the ISCR's diverse activities in FY 2005. For further information about the Institute, please contact us at the address below. Inquiries about how you might enhance the ongoing FY 2006 program at the ISCR, or beyond, are welcome.

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Exploratory Research in the Institutes

The ISCR supported three Exploratory Research in the Institutes (ERI) projects with Laboratory Directed Research and Development (LDRD) funds during FY 2005. These research grants are awarded to LLNL staff with the goal of developing ties to academia through co-funded research projects. Anticipating the emergence of data science as a cross-disciplinary theme, the ISCR has concentrated its efforts on developing technologies for large-scale and distributed datasets for the past several years. The current portfolio contains three projects covering a diverse range of topics, from providing a single interface to diverse data sources on the Web, to tracking objects in a succession of images, to a multi-resolution representation of scientific datasets for scalability across a range of computer architectures. This portfolio, originally motivated by purely scientific applications, has already paid dividends in some of LLNL's new homeland security applications.

Enabling Large-Scale Data Access

Principal Investigator

Chandrika Kamath, CASC

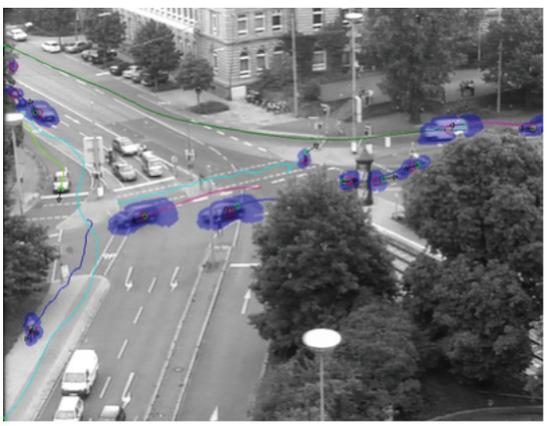
In this project, we are developing robust, accurate, and near-real-time techniques for detecting and tracking moving objects in video from a stationary camera. These techniques allow us to model interactions among the objects, thereby enabling us to identify normal patterns and detect unusual events. Our algorithms and software include techniques to separate the moving foreground from the background, extract features representing the foreground objects, track these objects from frame to frame, and postprocess the tracks for display. The project focuses on video taken under less-than-ideal conditions with objects of different sizes moving at different speeds, occlusions, changing illumination, poor weather, low resolution, and low frame rates.

To address these situations, this project enhances existing algorithms, which allows us to better understand their limitations. This, in turn, determines the conditions under which successful surveillance is possible. The algorithms and software are also being applied to spatiotemporal data from computer simulations and can be used to mine text, audio, image, and video data simultaneously.

In FY 2005, we

- Put together a data pipeline to allow us to experiment with different algorithms in each step of the pipeline
- Demonstrated our approach by successfully tracking in low-resolution, low-frame-rate video
- Reduced the computation time for the use of salient regions in tracking
- Obtained a better understanding of which methods work well under what circumstances and the sensitivity of each method to the settings of various parameters
- Filed a patent on our new approach to detection of moving objects.

In addition, a summer student from UCLA worked on developing a graphical interface enabling us to determine how the intensity of a pixel in a video frame varied over time. We also continued our interactions with UC San Diego on the problem of tracking under occlusions.



Tracks created using our tracking pipeline for a video of a traffic intersection. Some of the tracks are of objects that have moved out of the scene, for example, the green track at the top and the light blue track on the left.

Parallel Graph Algorithms for Complex Networks

Principal Investigators

Tina Eliassi-Rad, Keith Henderson, Scott Kohn, Andy Yoo, CASC

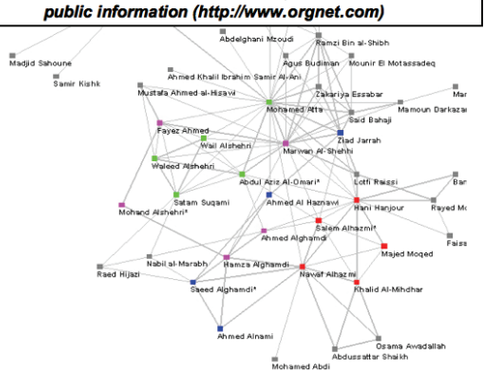
The intelligence community collects enormous amounts of data. Analysts must sift through this information and understand the interactions among individual pieces or subsets of data to identify potential threats. To facilitate this process, we are developing parallel and scalable algorithms for searching very large semantic graphs that will enable graph searches on distributed parallel computers. We anticipate significant decreases in parallel communication time by using edge partitioning and reductions in search complexity by using heuristic searches. The project has two aspects: (1) develop efficient parallel implementations using innovative data structures and algorithms, and (2) develop algorithms that exploit the structure of semantic networks.

Semantic graphs are used to encode relationship data gathered by intelligence agencies for counterterrorism purposes. By exploiting the large aggregate memory of parallel computers, this research will enable the complex network applications relevant to LLNL's national and homeland security missions to be scaled to unprecedented sizes. In addition, such parallel algorithms will also have applications in complex networks in other disciplines, particularly the analysis of metabolic networks in support of LLNL's mission in bioscience.

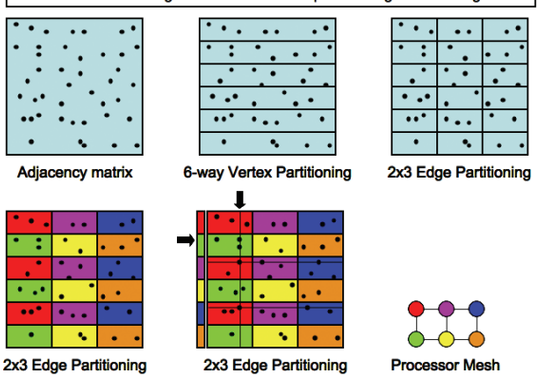
We have developed algorithms and approaches for analyzing and searching semantic graphs of more than a billion nodes using many thousands of processors. This work demonstrates that parallel computers can support very large semantic graphs. We anticipate that next-generation semantic-graph architectures will be based on these parallel computing ideas.

We report two main accomplishments in FY 2005. First, we developed a new innovative parallel graph search algorithm for finding paths in massive semantic graphs. Running on 32,000 nodes of the BlueGene/L supercomputer, the code required only a few seconds to search a graph with 3.2 billion vertices and 32 billion edges, the largest graph ever explored by any graph search method. This work was nominated for a Gordon Bell Prize at Supercomputing 2005. We also created new graph metrics and probabilistic models based on the semantic graph ontology. Our methods allow us to infer the existence of links and subgraphs in semantic graphs, which reduces the cost of point-to-point searches and enables analysts to detect patterns in the semantic graph.

Portion of the 9/11 Terrorist Network, constructed from public information (http://www.orgnet.com)



Goal: Partition graph to minimize processor communication while maintaining load balance. Example: 2D Edge Partitioning.



Effective and Reliable Data Exploration via Multiscale Morse Analysis and Combinatorial Information Visualization

Principal Investigator

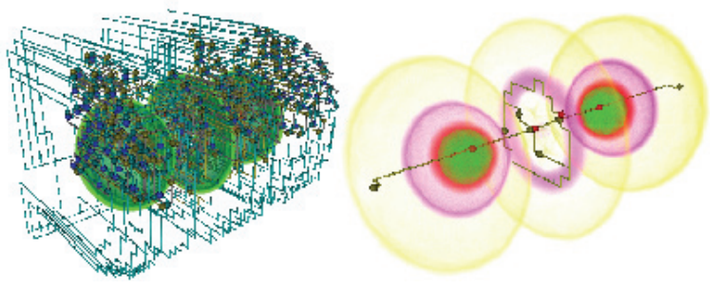
Valerio Pascucci, CASC

We are developing a new visualization framework based on general-purpose data-analysis tools coupled with information visualization techniques. The framework will allow fast computation and effective display of metadata roadmaps guiding the exploration of terabytes of raw data. We are using Morse analysis to build multiscale models of fundamental structures that are ubiquitous in scientific data. The large size and complexity of the topology graphs obtained will require new and general multiscale graph models that we will apply to the exploration of other combinatorial models. The environment will use progressive rendering of multiple linked views and present the graphs with context information that improves the overall data exploration and understanding process.

The success of this project will yield new data-exploration modalities for smooth and discrete data. At the scientific level, this will contribute to new basic research both in information visualization and in topology-based data analysis. In these areas, we will develop new multiresolution representation models, external memory algorithms and data structures. On a practical level, our technology will allow us to develop tools for data analysis and presentation that will improve the effective speed of accessing the information stored in terascale scientific data sets and in large semantic graphs. This will be accomplished both by increasing performance of the display methods and by integrating multiple presentation modalities for improved data understanding.

In FY 2005, we developed some of the core software tools and published the results in seven refereed papers that appeared or will appear in major visualization-oriented conferences. In particular, we have (1) constructed simplified topologies with tight error bounds, (2) constructed robust Jacobi sets for 2D scalar fields, (3) computed integrals on the Jacobi sets to evaluate the correlation between 2D fields, (4) demonstrated the robust computation of critical points in 3D sampled data, (5) implemented a framework with linked views coordinating multiple presentation modalities; (6) scaled the interface for the external memory visualization of large graph, and (7) completed the definition of data layout and file formats for storing large graphs that cannot fit in main memory.

In FY 2006, we will extend the 2D techniques to the volumetric case and work on a complete and robust computation of the 3D Morse complex with the main goal of testing time simplification of the Jacobi sets over time. Specifically, we will (1) use topological analysis to segment bubble structures in mixing fluid dynamics simulations; (2) use time tracking to provide detailed information and global summaries describing turbulent mixing behavior; (3) start integrating the topology components with the visualization framework based on linked views; and (4) start extending the tree visualization tools to the case of general graphs, first introducing a moderate number of cycles and then scaling to unconstrained connectivity.

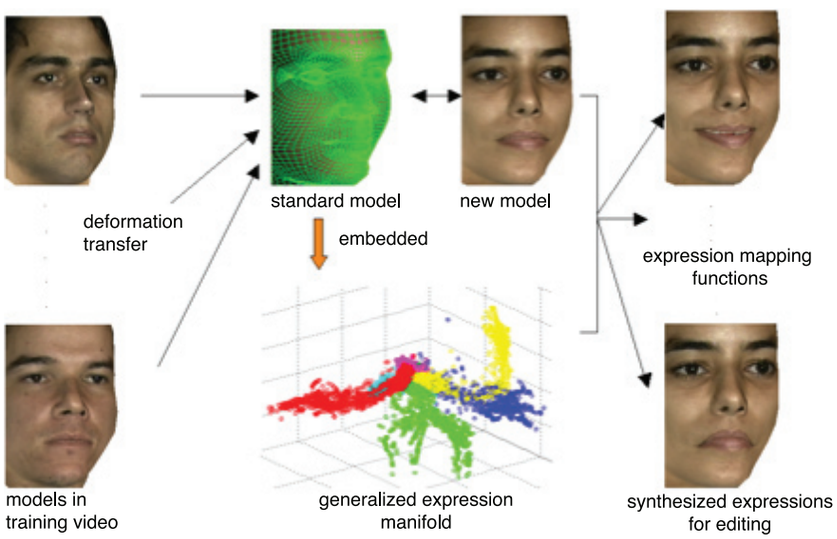


Topological analysis applied to the electron density distribution of a hydrogen atom under an intense magnetic field. Critical points and their connection in the full-resolution 3D Morse–Smale (left), and a simplified complex obtained by repeated cancellation of minimum persistence features. The main structures in the data are extracted naturally.

University Collaborative Research Program

The ISCR supported seven University Collaborative Research Program (UCRP) projects during FY 2005 at the University of California campuses that support graduate students working on doctoral thesis research. Along with their faculty principal investigators, the students work closely with an LLNL collaborator. The projects in FY 2005 spanned four different UC campuses, as well as the departments of civil engineering, computer science, mechanical engineering, and physics. They ranged from understanding and optimizing the performance of advanced architecture computers, to improving engineering simulation models, to developing object tracking and recognition, to basic computational science at the frontier.

Professor Matthew Turk of UC Santa Barbara, with LLNL co-investigator Lenny Tsap, worked on machine recognition of human expression (below). The focus is on computer vision technologies that are applied to applications in biometrics and interactive visualization. Computer vision is a promising and powerful sensing modality that can be used to unobtrusively track, model, and classify human appearance and behavior with direct applications to biometrics and interactive visualization systems. During the past year, progress was made in facial expression analysis, extracting and using reliable depth edges in images and video, as well as multimodal biometrics. In facial-expression analysis, the investigators represent high-dimensional face information in low-dimensional manifolds to investigate the representation and recognition of dynamic facial expressions.



Reports for the projects in the following table have been omitted from the printed version of the ISCR Annual Report in the interest of space, but can be found on the accompanying Web site. You can also obtain a CD-ROM containing these reports by calling (925) 422-1842.

University Collaborative Research Program, Fiscal Year 2005

Principal Investigator, Affiliation	Project Title	LLNL Contact
Scott Baden, UC San Diego	Data-Driven Execution of Communication-Tolerant Algorithms	Dan Quinlan, CASC
Serge Belongie, UC San Diego	A Regularization-Based Approach to Nonrigid Structure from Motion	Chandrika Kamath, CASC
Said Elghobashi, UC Irvine	DNS and Modeling of Dispersion of Solid or Liquid Particles in Turbulent Flows	Robert Lee, Atmospheric Sciences
Warren Pickett, UC Davis	Coexisting Superconductivity and Ferromagnetism: Applications to Real Materials	Francois Gygi, CASC
Mark Rashid, UC Davis	Lagrangian Simulation of Penetration and Other Extreme-Deformation Events: Moving Beyond Meshless Methods	Mike Puso, Engineering
Allen Snavely, UC San Diego	Memory Access Pattern Signatures and Certificates of Relevance for Benchmarks	Bronis de Supinski, CASC
Matthew Turk, UC Santa Barbara	Visual Tracking and Recognition for Biometrics and Interactive Visualization	Lenny Tsap, Electronics Engineering Technologies

University Subcontracts

The ISCR supported 24 research subcontracts to various institutions throughout the United States. These contracts are normally funded by programs at LLNL to help address long-term Laboratory requirements. They typically fund residential visits research by university faculty and students for in close collaboration with scientists in the Computation Directorate.

Professor Kwan-Liu Ma of UC Davis develops advanced visualization technology for the Computer Incident Advisory Capability (CIAC) at LLNL. The mission of CIAC is to apply cybersecurity expertise to prevent, detect, react to, and recover from cyber incidents for DOE/NNSA and other national stakeholders. The network data regularly collected by CIAC is not extensively exploited due to the enormous data size. Ma is investigating how visualization can effectively assist in the process of security data analysis and understanding. The study focuses on designing appropriate visual mapping of the data for different levels of abstraction and information seeking, providing the user with multiple linked views of the data along with intuitive interaction mechanisms, which can potentially increase CIAC's capability in timely detection and characterization of changing network activities. A port-data-visualization system demonstrates that a "drill-down" methodology works for finding network scans by applying it to a 24-hour-long dataset at a 10-minute resolution in the figure below.

Reports for the projects in the following table have been omitted from the printed version of the ISCR Annual Report in the interest of space, but can be found on the accompanying Web site. You can also obtain a CD-ROM containing these reports by calling (925) 422-1842.

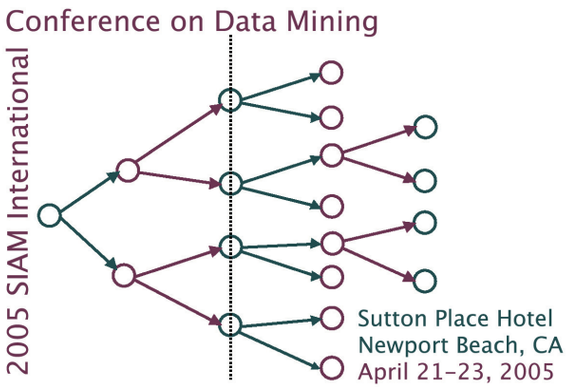
University Subcontracts, Fiscal Year 2005

Principal Investigator	Project Title	Institution
Dorian Liepmann	DNA Transport in Microfluidic Systems	UC Berkeley
Bernd Hamann	Topological Analysis for Scientific Visualization	UC Davis
Berni Alder	Investigation of Flow Instabilities at the Molecular Level	UC Davis
Greg Miller	A One-Dimensional Conservative Method for Front Tracking in a Compressible Medium	UC Davis
Kwan-Liu Ma	Advanced Visualization Technology for DOE/NNSA	UC Davis
Kwan-Liu Ma	Investigation of Flow Instabilities at the Molecular Level	UC Davis
Said Elghobashi	Numerical Simulation of Compressible Flow Past a Solid Sphere	UC Irvine
Ana Iontcheva	Element Agglomeration AMGe for Contact Problems	UC San Diego
Serge Belongie	Robust Multiple Object Tracking	UC San Diego
Jim Jones	Multigrid Approaches for Maxwell Equations	Florida Tech
John Ruge	Spectral AMGe, ALE3D & FOSPACK	Front Range Scientific Computations
Steve McCormick	FOSPACK, AMG, Adaptive AMG, Compatible Relaxation, Parallelization and Application Codes	Front Range Scientific Computations
Andrew Knyazev	Hypre for Symmetric, Generalized Eigenvalue Problems	Fusion Numerics, Inc.
Ludmil Zikatanov	Optimal AMG Interpolation and Convergence Theory	Penn State University
Don Schwendeman	Development of Numerical Methods for Mathematical Models of High-Speed Reactive and Nonreactive Flow	Rensselaer Polytechnic Institute
John Mellor-Crummey	Open Source Software Technology for Transforming Scientific Problems	Rice University
Raytcho Lazarov	Construction and Preconditioning of Finite Element Approximations of Mixed Problems	Texas A&M
Michael Bybee	Particle Interactions in DNA-Laden Flows	University of Illinois
David Jensen	Relational Pathfinding	University of Massachusetts
Dinesh Manocha	Cache-Oblvious Mesh Layouts	University of North Carolina
Claudio Silva	Studying of Topology of Point-Set Surfaces	University of Utah
Ellen Riloff	Bioforensics Text Extraction	University of Utah
Hans De Sterck	Improving Complexity of Parallel AMG	University of Waterloo
Jason Kraftcheck	Mesquite Software Development	University of Wisconsin

Workshops, Conferences, and Program Sponsorships

The ISCR co-sponsored eight off-site scientific workshops and conferences in FY 2005. These workshops were hosted in cooperation with other organizations, such as the Society for Industrial and Applied Mathematics (SIAM), the Institute for Pure and Applied Mathematics (IPAM), the Department of Homeland Security, and Argonne National Laboratory. Some ISCR workshops are one-of-a-kind exploratory workshops that assemble experts to scope out possible new programs. Others have become part of the fabric of their disciplines and are held at regular intervals. In each case, there is a vital LLNL interest and typically, several Laboratory researchers participate.

Chandrika Kamath of LLNL co-chaired the 5th SIAM International Conference on Data Mining, held in Newport Beach, California, in April 2005. This conference, which SIAM adopted after Kamath and early collaborators pioneered it as a workshop at the University of Minnesota, continued the tradition of providing an open forum for the presentation and discussion of innovative algorithms, as well as novel applications of data mining. The number of paper submissions this year surpassed all previous years, indicating that the conference is becoming established in the data-mining community. This year's conference was also co-sponsored by the American Statistical Association, which encouraged strong participation by statisticians. Workshops within the conference covered a range of topics, including Data Mining in Sensor Networks to Link Analysis, Feature Selection, Clustering, High-Performance Mining, and Mining Scientific and Engineering Datasets. The conference attracted many students from UC San Diego, UCLA, and UC Santa Barbara, as well as a mix of attendees from academia, industry, and national laboratories.



The reports listed in the following table have been omitted from the printed version of the ISCR Annual Report in the interest of space, but can be found on the accompanying Web site. You can also obtain a CD-ROM containing these reports by calling (925) 422-1842.

Workshops, Conferences, and Program Sponsorships, Fiscal Year 2005

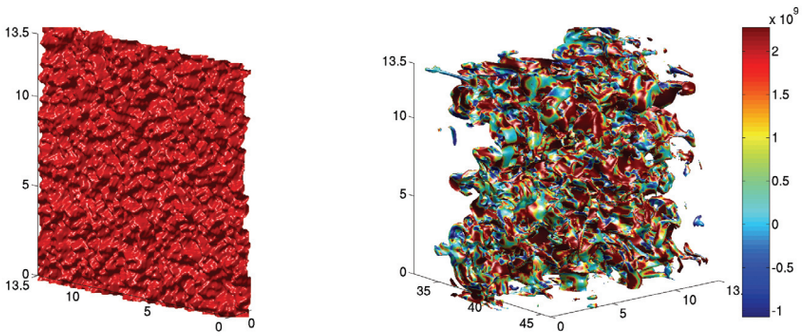
Title	Location	Dates
Workshops and Conferences		
7th Overset Composite Grid and Solution Technology Conference	Huntington Beach, CA	Oct 5–7, 2004
16th International Conference on Domain Decomposition Methods	New York, NY	Jan 12–15, 2005
12th Copper Mountain Multigrid Conference	Copper Mountain, CO	Apr 3–8, 2005
5th SIAM International Conference on Data Mining	Newport Beach, CA	Apr 21–23, 2005
2005 International Conference on Preconditioning Techniques for Large-Space Matrix Problems in Scientific and Industrial Applications	Atlanta, GA	May 19–21, 2005
Householder Symposium XVI: The Householder Meeting on Numerical Linear Algebra	Champion, PA	May 23–27, 2005
AMG/FOSLS Summit	Lake City, CO	Sep 12–18, 2005
8th European Multigrid Conference	Sheveningen, The Netherlands	Sep 27–30, 2005
Program Sponsorship		
UCLA Institute for Pure and Applied Mathematics, Research in Industrial Projects for Students	Los Angeles, CA	Jun 27–Aug 27, 2005

Summer Research Program

The ISCR's summer visitor program for FY 2005 was its second largest ever with approximately 100 students in residence, as well as 11 faculty members. Students are assigned individual LLNL mentors and given specific projects, ranging from programming tasks to original research, to which they will contribute based on their background and skills.

Marco Latini from Cal Tech spent the summer of 2005 working with Oleg Schilling of LLNL's AX Division on turbulent transport in a Richtmyer–Meshkov instability (RMI). The RMI develops at a surface separating two gases following the passage of a shock. In order to accurately characterize the development of the turbulent mixing layer, appropriate initial conditions are needed. Latini investigated initial conditions using stochastic noise that follows a prescribed perturbation spectrum that was taken from studies of surface perturbations on internal confinement fusion capsules and is used to break symmetry and to accelerate the development of turbulence. The new capability is used to study the effects of initial conditions on the development of the layer and to guide the development of turbulent transport models for Richtmyer–Meshkov flows.

Presented below is a visualization of the mass-fraction isosurface corresponding to the new initial conditions (left) and the evolution of the instability at 5ms following the passage of the shock and displaying the complex structure of the flow. The color represents the values of the vortex stretching, which is used to characterize turbulent flows (right).



Reports for the projects in the following table have been omitted from the printed version of the ISCR Annual Report in the interest of space, but can be found on the accompanying Web site. You can also obtain a CD-ROM containing these reports by calling (925) 422-1842.

Name, Affiliation	Project Title	Mentor, Host Organization
Sabbatical Visitors		
Jeff Buckwalter, University of San Francisco	Queuing Network Models of Performance of High-End Computing Systems	Bronis de Supinski, CASC
Thomas Hagstrom, University of New Mexico	High-Order Structured Grid Methods for Wave Propagation on Complex Unbounded Domains	William Henshaw, CASC
Karen L. Karavanic, Portland State University	ASCI Simulation Development Environments	John May, CASC
Sally McKee, Cornell University	Efficiently Exploring Architectural Design Spaces via Predictive Modeling	Bronis de Supinski, CASC
Summer Faculty		
Zhiqiang Cai, Purdue University	Multigrid, Mixed Finite Element, and Least-Squares Methods for Partial Differential Equations	Barry Lee, CASC
Timothy Chartier, Davidson College	Adaptive Multigrid and Page Rank Computation	Van Emden Henson, CASC
Clint Dawson, University of Texas at Austin	Discretizations and Splitting Methods for Radiation Diffusion and Compressible Flows	Carol Woodward, CASC
Irene Livshits, Ball State University	Multiscale Solvers for Schrodinger Equations	Rob Falgout, CASC
Anne Ngu, Texas State University	Scientific Process Automation	Terence Critchlow, CASC
Georgio Scorzelli, University of Roma Tre	Multiresolution Computation and Presentation of Contour Trees Streaming Computation of Reeb Graphs	Valerio Pascucci, CASC
Pete Wells, University of San Francisco	Third Sabbatical Leave from USF	Pat Miller, CASC
Summer Students		
Maria Luisa Alano, University of Chicago	SPEAR—A Fully Automated Python-Wrapping Generator for C Code	Pat Miller, CASC
Garrett Aldrich , UC Davis	Topology Imagery Conversion	Valerio Pascucci, CASC
Dustin Anderson, Cal Poly San Luis Obispo	Tasks Complete for ORAD and TAMM	Don MacQueen, CADSE
John C. Anderson, UC Davis	Visualization of Distribution-Field Datasets	Mark Duchaineau, CASC
Ben Apodaca, Northern Arizona University	J2EE Application Development	Karen DeHoyos, NIFE
Bradley Auble, BYU	Disk Image Deployment at the Computation Training Center	Paul Sanguinetti, ICCD
Abraham Bagherjeiran, University of Houston	Orbit Classification: A Graph-Based Approach	Chandrika Kamath, CASC
Jeffrey W. Banks, Rensselear Polytechnic Institute	Reactive, High-Speed Multi-Fluid Flows	William Henshaw, CASC
James Brannick, CU-Boulder	Compatible, Relaxation-Based Coarsening in AMG	Rob Falgout, CASC
Joseph Burks, Cal State Sacramento	Investigations for a Highly Parallel Image-Analysis Pipeline	Marcus Miller, CASC
Michael Bybee, University of Illinois	Particle Interactions in DNA-Laden Flows	David Trebotich, CASC
Steven Callahan, University of Utah	Progressive Volume Rendering of Unstructured Grids	Valerio Pascucci, CASC
Michael Casolary, University of the Pacific	Palm Conduit Development for the Macintosh, and Optimization of Monitoring Script	Gary Laguna, ERD
Paul Castellucci, Stanford University	Hybrid Turbulence Models for Massively Separated Flows	Rose McCallen, CASC
Christopher Chan, Princeton University	An Exploratory Study of Neural Networks for Function Approximation	Charles Tong, CASC
Jedidiah Chow, UC Berkeley	Simulating the Effects of Habitat Fragmentation on Population Persistence	Tanya Vassilevska, CASC
Kree Cole-McLaughlin, UCLA	Topological Analysis of High-Dimensional Datasets	Valerio Pascucci, CASC
William Conner, University of Illinois	Validation and Verification of an XML Interface	Terry Brugger, NAIC

Name, Affiliation	Project Title	Mentor, Host Organization
Dylan Copeland, Texas A&M University	Multigrid Methods for the Time-Harmonic Maxwell Equations	Barry Lee, CASC
Paul D'Avilar, Johns Hopkins University	Internet Ballistics—Retrieving Forensic Data from Network Scans	Tony Bartoletti, CIAC
Jose De Figueiredo Coutinho, Imperial College London	QRose: A Graphical User Interface Library for ROSE Source-to-Source Translators	Dan Quinlan, CASC
Garrett DeHoyos, Cal Poly San Luis Obispo	WTDR, CASTLE, SWP	Valerie Stanton, NIFE
Scott Dillard , UC Davis	Topological Visualization with Volume Rendering	Valerio Pascucci, CASC
James Doyle, Carnegie Mellon University	Detecting the Spread of Virus Emails	Barry Dahling, ITPD
Matthew Dyer, Louisiana State University	Targeting Unique Pathogen Signatures	Tom Slezak, EEBI
David Echeverria-Ciaurri, Centrum voor Wiskunde en Informatica	Towards Multilevel Optimization: Space Mapping and Manifold Mapping	Charles Tong, CASC
Emily Eder, UCLA	A Graphical Representation of Temporal Data from Simulations	Cyrus Harrison, CASC
Michael Elliott, University of San Francisco	Queuing Network Models of Performance of High-End Computing Systems	Bronis de Supinski, CASC
Pak-Wing Fok, MIT	Vortex Dynamics of Soapfilms	Petri Fast, CASC
Mark Gates, University of Illinois	User-Friendly Python Interface to ODE Solvers	Steven Lee, CASC
Attila Gyulassy, UC Davis	Topology-Based Simplification for 3D Scalar Field Visualization	Valerio Pascucci, CASC
Michelle Hallikainen, UCLA	The California Electrical Economy and Nuclear Plant Relicensing	Alan Lamont, EEBI
Lyle Hansen, Las Positas Community College	JCATS Client Assistant Window with Emphasis on Information Fusion	Hal Brand, NAIC
Vera Hauge, University of Oslo, Norway	Program Slicing with ROSE	Dan Quinlan, CASC
W. Taylor Holliday, UC Davis	Combinatorial Morse Theory for Scientific Data Analysis	Valerio Pascucci, CASC
Gary Hon, UC San Diego	Improving vPCR	Shea Gardner, EEBI
Jason Howell, Clemson University	Solution Methods for Nonlinear Reaction–Diffusion Equations	Carol Woodward, CASC
David Hoyt, BYU	Countermeasures Test Bed	James Schek, NAI/HSO
Michael Huffman, Purdue University	Automated Regression Testing for Argus DBUI Using Eggplant	Dan Jones, EEBI
Lorenzo Ibarria, Georgia Tech	Structured Data Compression	Peter Lindstrom, CASC
Alin Jula, Texas A&M University	Automatic Detection of Hot Spots in C/C++ Programs	Dan Quinlan, CASC
Jason Kimball, UC Irvine	Large-Scale Atom Data Visualization	Mark Duchaineau, CASC
Bonnie Kirkpatrick, UC Berkeley	Clustering Proteins According to Structural Features	Carol Zhou and Adam Zemla, EEBI
Steven Ko, University of Illinois	Porting DPCL to BlueGene/L	Bronis de Supinski, CASC
Milind Kulkarni, Cornell University	AST Compression for Large-Scale Programs and Interprocedural Program Slicing with ROSE	Dan Quinlan, CASC
Marco Kupiainen, Royal Institute of Technology, Sweden	Embedded Boundary Method of Navier–Stokes Equations	Bjorn Sjogreen, CASC
Asher Langton, University of Wisconsin	Adding Cray Pointers to GNU Fortran	Mike Kumbera, AX Division
Ilya Lashuk, CU-Denver	A Spectral Element Agglomeration AMG Solver Using Element Topology and Element Matrices	Panayot Vassilevski, CASC
Marco Latini, Cal Tech	Turbulent Transport Properties of Three-Dimensional Multimode Reshocked Richtmyer–Meshkov Instability	Oleg Schilling, AX Division
Greg Lee, UC San Diego	Porting the Dynamic Probe Class Library to BlueGene/L	Bronis de Supinski, CASC Martin Schulz, CASC Dong Ahn, ICCD

Summer Research Program

Name, Affiliation	Project Title	Mentor, Host Organization
Brian Lum, UC San Diego	SynGoogle: A Tool for Enhanced Searching	Julie Pitt, EEBI
Eric Machorro, University of Washington	Numerical Methods for the 1D Spherical Neutron Transport Equation	Britton Chang, CASC
Michael Maire, UC Berkeley	Tracking Vehicles in Traffic Surveillance Video	Chandrika Kamath, CASC
Heather Maldonado, Northern Arizona University	Livermore Computing Forms Reconstructing	Renee Silva, ICCD
Daniel May, Mississippi State	A GPU-Accelerated Speech Recognition System	John Johnson, CASC
Dmitry Morozov, Duke University	From Vineyards to Simplification	Valerio Pascucci, CASC
James Muehlner, UC Davis	CAR Survey Maker	Jason Conkey, CADSE
Mike Noeth, North Carolina State	Implementation of PAPI 3.0.8.1 on BlueGene/L	Bronis de Supinski, CASC
Joshua Nolting, CU-Boulder	Implementing A Parallel Version of FOSPACK	Ulrike Yang, CASC
Timothy Paik, UC Berkeley	Subspace Detector Design Tool	David Harris, EEBI
Guy Pavel, Granada High School	NIFE Intern	Stanley Stone, NIFE
Christophe Picard, University of Houston	Domain Decomposition Methods and Deforming Boundary Simulation Using Overset Grids	Petri Fast, CASC
Peter Pirkelbauer, Texas A&M University	Crossing the Mississippi Twice— Bridging the Gap Between ROSE and the Pivot	Dan Quinlan, CASC
Jonathon Poling, George Washington University	Subnet-Directorate Mapping in the Vulnerability Tracking Database and Evaluating Pro Discover Forensic Software	Barry Dahling, LSD
Raymond Pon, UCLA	Defining and Measuring the Interestingness of Documents	Terence Critchlow, CASC David Buttler, CASC
Radu Popovici, Cornell University	Tools for Static Analyses	Dan Quinlan, CASC
Oliver Rheinbach, Universität Duisburg-Essen, Campus Essen	Using Hypre for the FETI-DP Coarse Problem	Panayot Vassilevski, CASC
George Roberts, Georgia Tech	Cluster-Based Image Segmentation	Chandrika Kamath, CASC
Terri Roberts, Las Positas Community College	Biosciences Computer Security Certification and Accreditation (C&A)	David Ow, EEBI
Clay Ross, Las Positas Community College	Space Action Team Photo Management	Paul Corrado, Plant Engineering
Barry Rountree, University of Georgia	Porting DynInst to BlueGene/L	Bronis de Supinski, CASC
Geoff Sanders, CU-Boulder	A Multilevel Eigensolver for Adaptive Algebraic Multigrid	Panayot Vassilevski, CASC
Rahul Satija, Duke University	Genomic Sequences to Identify Important DNA Polymorphisms	Tom Slezak, EEBI
Carlos Scheidegger, University of Utah	Studying the Topology of Point-Set Surfaces	Valerio Pascucci, CASC
Jessica Schoen, UC Berkeley	Extending EMSolve, An Electromagnetics Code	Mark Stowell, CADSE
Brendan Sheehan, CU-Boulder	Multigrid Methods for Neutron Transport	Britton Chang, CASC
Alex Sherman, Columbia University	Efficient, Out-of-Core Data-Access Methods for Volumetric and High-Definition Image Data	Valerio Pascucci, CASC
Nija Shi, UC Davis	Wrapping CALE Commands Using SWIG	Paul Amala, AX Division
Nija Shi, UC Davis	Supporting RMI for BABEL	Gary Kumfert, CASC
Karan Singh, Cornell University	Performance Analysis and Prediction	Bronis de Supinski, CASC
Jonathan Strasser, UC Davis	Robust Testing of Distributed Multilayered Image Cache	Valerio Pascucci, CASC
Valerie Szudziejka , UC Davis	Streaming Computation of Reeb Graphs	Valerio Pascucci, CASC

Name, Affiliation	Project Title	Mentor, Host Organization
Erika Tarte, UC Berkeley	SDCSI	David Gutierrez, NIFE
Brian Tran, Stanford University	Extracting Useful Information from Complex Data	Norman Franke, NAIC
Mark Vickers, BYU	Verification & Validation Python-Based Web Service for DakTools	George Christianson, DCOM
Huy Vo, University of Utah	High-Performance External Sort, and Streaming Simplification of Tetrahedral Meshes	Valerio Pascucci, CASC
Bei Wang, UC Davis	Adaptive Particle-Refinement Method in Smoothed-Particle Hydrodynamics	Garry Rodrigue, ISCR
Chunbo Wang, Purdue University	A Parallel-Finite Element Method for the Pseudostress-Velocity Form Stokes Equations — Multigrid Solution Built on SAMRAI	Brian Gunney, CASC
Vincent Weaver, Cornell University	Development of a Cache-Conflict Analysis Tool	Martin Schulz, CASC
Brian White, Cornell University	Towards Abstraction Optimization Through Generalized Compiler Transformations	Dan Quinlan, CASC
Daniel Wilhelm, Purdue University	ViSUS Package for Yorick	Steve Langer, AX Division
Tim Wong, UC Davis	Work Order System and Livermore Account Management System	Ken Sumikawa, NAIC
Guangri Xue, Penn State University	Robust Numerical Algorithm for the Proton Exchange Membrane Fuel Cell Modeling and Related Multigrid Methods	Rob Falgout, CASC
Sung-Eui Yoon, University of North Carolina	Comparing Layouts of Polygonal Meshes and Related Multigrid Methods	Peter Lindstrom, CASC
Yongquan Cathy Yuan, Indiana University	MATLAB Bindings for Babel	Tom Epperly, CASC
Rafal Zboinski, Georgia Tech	A 3D Visualization and Modeling Framework for NIF Target Area Systems	Kelley Herndon Ford, NIFE
Shun Zhang, Purdue University	Distributive Relaxation for Saddle Point Problems	Panayot Vassilevski, CASC
Yuan Zhao, Rice University	Parameterized Loop Fusion for Automatic Performance Tuning	Dan Quinlan, CASC

Seminar Series

The ISCR hosted 81 seminars from visitors in FY 2005 covering a wide spectrum of research areas and recruited an additional 22 speakers from LLNL's ranks to address visiting students.

The ISCR Summer Student Lecture Series was established in 2000 and evolved into two different series in Summer 2005—Internships in Computational Modeling at the Terascale (ICMT) and Internships in Computer Science at the Terascale (ISCT).

The ASC Institute for Terascale Simulation Lecture Series (ITSLS) was also established in 2000 to enrich the intellectual atmosphere of LLNL's largest simulation community through the visits of leaders representing the diverse areas of computation. In FY 2005, we hosted C. William Gear, Ken Kennedy, Jeff Hawkins, Jack Dongarra, and Alfred V. Aho.

Professor Al Aho of Columbia University (below) delivered his ITSLS talk, "Can We Get Reliable Programs from Unreliable Programmers?," to a standing-room-only audience on July 22, an event that was rebroadcast on Lab television for two weeks after his visit. His talk reviewed the challenges of making software reliable and strides made to detect and prevent programming bugs to ward off hostile attacks.

Aho is best known as the author of 10 textbooks, including volumes of the computer science canon on compilers, data structures, programming languages, and discrete algorithms. Much of the computing infrastructure we take for granted, namely the UNIX operating system and the C and C++ programming languages, is due to Aho and his former colleagues in the Computing Sciences Research Center at Bell Laboratories, which Aho joined in 1967 and ultimately served as director. In 1999, Aho was elected to the National Academy of Engineering.

Seminar abstracts listed in the following table have been omitted from the printed version of the ISCR Annual Report in the interest of space, but can be found on the accompanying Web site. You can also obtain a CD-ROM containing these abstracts by calling (925) 422-1842.

Seminar Series

Name, Affiliation	Seminar Title	Date
ITS Lecture Series		
C. William Gear, University of Illinois	Projective Integration Methods for Multiscale Problems	10/19/04
Ken Kennedy, Rice University	Compilers for High-Performance Computer Systems: Do They Have a Future?	12/7/04
Jeff Hawkins, Redwood Neuroscience Institute	A New Theory of Neocortex and its Implications for Machine Intelligence	3/1/05
Jack Dongarra, University of Tennesee	An Overview of High-Performance Computing and Self-Adapting Numerical Software	5/17/05
Alfred V. Aho, Columbia University	How Can We Get Reliable Software from Unreliable Programmers?	7/5/05
Faculty Seminars		
Simone Sbaraglia, IBM, T.J. Watson Research Center	pSigma: An Infrastructure for Parallel Application Performance Analysis Using Symbolic Specification	10/4/04
Alberto Paoluzzi, Third University of Rome, Italy University of Roma Tre	A Progressive Environment for Geometric and Physical Modeling	10/8/04
Elizabeth Simon, San Diego Supercomputer Center	Performance Prediction and Optimization Using the SDSC PMaC Framework	10/15/04
Stephen Scott, Oak Ridge National Laboratory	High Availability in High-Performance Computing	10/21/04
Antonino Ferrante, UC Irvine	Direct Numerical Simulation of Particle-Laden Turbulent Flow Over a Backward-Facing Step	10/28/04
Allen Malony, University of Oregon	Performance Technology for Productive, High-End Parallel Computing	10/29/04
Izaskun Garrido, Centre for Integrated Petroleum Research	Modeling Multiphase Flow in Porous and Fractured Media	11/4/04
Juergen Geiser, Weierstrasse Institute for Applied Analysis and Stochastics	Simulations in Crystal Growth for SiC Single Crystal: Numerical Methods and Applications	11/11/04
Serge Belongie, UC San Diego	Behavior Recognition via Spatio-Temporal Features	11/12/04
Andrew McCallum, University of Massachusetts	An Introduction to Information Extraction with Conditional Random Fields	11/16/04
Umit Catalyurek, Ohio State University	Runtime and Compiler Support for Large-Scale, Data-Driven Science	11/17/04
Clint Dawson, University of Texas at Austin	Discretization Techniques for Coupled Flow and Transport	11/18/04
Michael Garland, University of Illinois	Harmonic Functions for Quadrilateral Remeshing of Arbitrary Manifolds	11/19/04
Jacob Sorensen, UC San Diego	Tarragon: Asynchronous Data-Driven Execution of Parallel Programs	11/30/04
John Feo, Cray, Inc.	Cray Eldorado — Hardware and Performance	12/1/04
Concettina Guerra, University of Padova	Structural Analysis in Computational Biology	12/3/04
Dhabaleswar Panda, Ohio State University	Designing Next Generation High-Performance Clusters and Datacenters with InfiniBand	12/6/04
Mayya Tokman, UC Berkeley	Faster Integration of Stiff Systems of ODEs with Exponential Propagation Iterative (EPI) Methods	12/6/04
Kevin McCurley, IBM Almaden Research Center	Connection Subgraphs in Social Networks	12/8/04
Mikhail Shashkov, Los Alamos National Laboratory	Mimetic Finite Difference Methods for Partial Differential Equations and Discrete Vector and Tensor Analysis	12/9/04
Keshav Pingali, Cornell University	A Semi-Automatic System for Application-Level Checkpoint/Recovery (CPR)	12/10/04

Name, Affiliation	Seminar Title	Date
Alan Kyker, UC Davis	Numerical Study of Coexistence of Superconductivity and Ferromagnetism	12/15/04
Ellen Riloff, University of Utah	Weakly Supervised Learning Methods for Information Extraction from Narrative Text	1/6/05
Scott Margolis, Compuware Corp.	Risk-Based Testing in Software Development	1/11/05
Nedialko Nedialkov, McMaster University	Solving DAEs by Taylor Series	1/20/05
Gustavo Alonso, Swiss Federal Institute of Technology	Infrastructure for Virtual Laboratories	1/25/05
Allan Snavely, UC San Diego / San Diego Supercomputer Center	Performance Evaluation and Prediction for High-Performance Computing	2/1/05
Michael McCracken, UC, San Diego	Performance Evaluation and Prediction for High-Performance Computing	2/1/05
BaiLian Larry Li, UC Riverside	Ecological Complexity and Scaling	2/3/05
Anthony Yezzi, Georgia Tech	Visual Tracking with Active Contours and PDEs	2/24/05
Frank Mueller, North Carolina State	A Hybrid Hardware/Software Approach to Efficiently Determine Cache-Coherence Bottlenecks on the Itanium-2	3/9/05
Michael Franklin, UC Berkeley	HiFi — An Architecture for Large-Scale Sensor Data Processing	3/10/05
Bjorn Engquist, University of Texas at Austin	Heterogeneous Multiscale Methods	3/11/05
Bradford Chamberlain, Cray, Inc.	An Introduction to Chapel: Cray Cascade's High-Productivity Language	3/18/05
Neil Yorke-Smith, SRI International	Reliable Network Traffic Inference: A Constraint Programming Approach	4/19/05
Thomas Panas, Vaxjo University, Sweden	VizzAnalyzer: A Framework for Reverse Engineering Tool Construction	4/25/05
J. Walter Larson, Argonne National Lab	The Parallel Coupling Problem and the Model Coupling Toolkit	4/26/05
Andreas Saebjornsen, University of Oslo	Visualization of Complex Heap-Based Data Structures	4/29/05
Ivan Yotov, University of Pittsburgh	Multiphysics Couplings of Subsurface and Surface Flows	5/2/05
David Maier, Portland State University	Keeping the Columbia Flowing: Managing the Data from an Environmental Observation and Forecasting System	5/5/05
Kirk Cameron, University of South Carolina	High-Performance, Power-Aware Distributed Computing	5/9/05
Barbara Chapman, University of Houston	OpenMP: Where Are We Headed?	5/10/05
Eunjung Lee, CU-Boulder	FOSLL* Method for Eddy Current Problem with Three-Dimensional Edge Singularities	5/18/05
Eric Darve, Stanford University	Computational Molecular Modeling: Algorithms and Computer Hardware	5/19/05
James Dehnert, Transmeta Corp.	The Transmeta Crusoe: VLIW Embedded in CISC	5/20/05
Claudio Silva, University of Utah	Point-Set Surfaces: An Update and Recent Work	5/20/05
Zhendong Su, UC Davis	Research on Software Reliability and Security	5/24/05
John Mellor-Crummey, Rice University	Cross-Architecture Performance Predictions for Scientific Applications Using Parameterized Models	5/27/05
Robert Fowler, Rice University	HPCToolkit: The Rice Performance Tools	5/27/05
Shmuel Ur, IBM	Testing Multithreaded Applications with ConTest	6/1/05
Shmuel Ur, IBM	Code Coverage	6/2/05
Salim Hariri, University of Arizona	Autonomic Computing: The Next Era to Design and Program High-Performance Computing Systems and Applications	6/3/05

Seminar Series

Name, Affiliation	Seminar Title	Date
H.C. Yee, NASA Ames Research Center	Nonlinear Filtering and Limiting in High-Order Methods for Ideal and Non-Ideal MHD	6/7/05
Gregory Richard Watson, Los Alamos National Laboratory	The Eclipse Parallel Tools Platform	6/8/05
Walter Burkhard, UC San Diego	Archival Storage Data Layouts and Algorithms	6/8/05
Adrian Bejan, Duke University	Constructal Theory of the Generation of Flow Configuration	6/9/05
Lyle Ungar, Universtiy of Pennsylvania	Dynamic Feature Generation and Selection in Multirelational Learning	6/13/05
Valerie Taylor, Texas A&M University	Analysis and Modeling of Parallel and Distributed Applications	6/14/05
Norden E. Huang, NASA Goddard Space Flight Center	Data Mining in this Nonlinear and Nonstationary World: What We Should Look For, and How?	7/14/05
Anil Deane, University of Maryland	Numerical Methods for Space Plasma Physics	7/21/05
Adam Landis, Parasoft, Inc.	Increasing Software Quality Through Automated Error Prevention (AEP)	7/26/05
Larry Johnsen, Parasoft, Inc.	Increasing Software Quality Through Automated Error Prevention (AEP)	7/26/05
Rod Oldehoeft, Los Alamos National Laboratory	OpenHPC: Supporting Open-Source Software in High-Performance Computing	7/28/05
David L. Wray, North Carolina Department of Agriculture	Using the North Carolina Multi-Hazard Threat Database for Homeland Defense	8/1/05
Katie Antypas, University of Chicago	FLASH Code Version 3	8/4/05
Cyrus Shahabi, USC	Wavelets and Web Services (W2) for Online Scientific Data Analysis	8/4/05
Samuel Feng, Rice University	Discontinuous Galerkin Methods for the 1D Spherical Neutron Transport Equation	8/10/05
Kevin Skadron, University of Virginia	Physical Constraints and the Design of Multi-Core Chips	8/10/05
Peter Szwed, Cornell University	Going Native: Faster Architectural Simulation Fast-Forwarding	8/12/05
Johannes Kraus, Austrian Academy of Sciences	An Edge-Based Algebraic Multigrid Method for Finite-Element Elasticity Problems	8/16/05
Karen Karavanic, Portland State University	The PerfTrack Performance Experiment Management Tool	8/18/05
Robert C. Kirby, University of Chicago	The FEniCS project: Automation and Algorithms for Finite Element Methods	8/22/05
Dan Roth, University of Illinois	Learning and Inference for Natural Language Processing and Intelligent Access to Information	8/29/05
Donna Calhoun, University of Washington	Wave Propagation Algorithms and Adaptive Mesh Refinement on Quadrilateral and Hexahedral Grids	9/8/05
Nikolaos Nikiforakis, University of Cambridge	Towards a Next-Generation Climate Model	9/16/05
Sameer Shende, University of Oregon	TAU: Performance Technology for Productive, High-Performance Computing	9/28/05

Summer Lecture Series

Name, Affiliation	Seminar Title	Date
Steven F. Ashby, CAR	Welcome to LLNL and CAR	6/14/05
Karen L. Karavanic, Collaborator	Performance Measurement and Analysis for High-End Computing	6/15/05
Bill Henshaw, CAR / CASC	Solving PDEs on Moving and Adaptive Overlapping Grids	6/21/05
Chandrika Kamath, CAR / CASC	Scientific Data Mining: The Sapphire Project	6/22/05
Steven Lee, CAR / CASC	Projective Integration Methods for Multiscale Problems	6/28/05
Dave Wiltzius, ICC / Mgmt. and Admin	Research and Advanced Network Efforts at LLNL	6/29/05
Gary Kumfert, CAR / CASC	Power Presentations	7/12/05
Robert Ferencz, Engineering **Mike Puso**, Engineering	Computational Engineering "HOT TOPICS"	7/19/05
Barna Bihari, CAR / CASC	Transport Methods	7/26/05
Terry Brugger, CAR / NAIC	Computer Security	7/27/05
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