Where

high-performance

solution

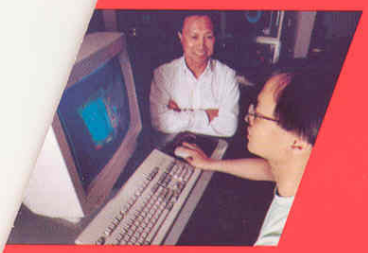
meets

bottom-line

objective

The Applications Department

Cray Research, Inc.



The Applications Department

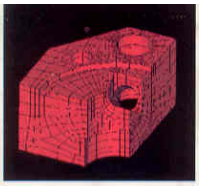
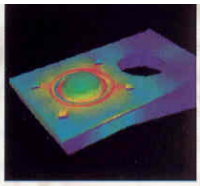
Cray Research, Inc.

By simulating an entire processing plant on a Cray Research supercomputer, German chemical company Bayer AG increased plant capacity and developed a completely new control strategy that significantly reduced energy use—all with little capital invested.

Cray Research applications experts have designed a new software module that allows for "design of experiments" in plastic injection molding problems. The major U.S. car companies estimate that eliminating just one trial run for a single mold could save as much as $40,000 and six weeks of time.

A provider of services and custom software for all major American automobile companies, Altair Engineering keeps its four-processor CRAY EL system busy with crash and bumper analysis, structural analysis of vibrations and passenger fatigue, and structural optimization for the shape and size of cars. With some configurations priced as low as $150,000, the CRAY EL90 product line makes supercomputing more affordable; more than 180 of these compact, air-cooled supercomputing systems are installed worldwide.

Applications

VALUE

Value. Return on investment. Timely answers to the real-world questions that stand between you and bringing your product to market or your project to completion. With its focus on high-performance application programs that run on Cray Research platforms from compact, air-cooled systems to the top-of-the-line CRAY C90 system and massively parallel processing CRAY T3D system, the Cray Research Applications Department ensures that Cray Research customers achieve their technical and business objectives.

With first-hand industry experience from organizations such as Siemens, Ford Motor Company, Renault, Apple Computer, Fujitsu, Amoco, Texaco, Air Products, and many other companies, the 80-plus members of the Applications Department in Eagan, Minnesota, understand the challenges today's businesses face. As specialists in their engineering and scientific disciplines and experts in the use of Cray Research supercomputing technology, these same applications analysts are well-positioned to make a difference in meeting and overcoming those challenges.

Our experience is your advantage

- Special I/O routines to take advantage of Cray Research's unique I/O power
- Highly optimized vector and parallel numeric kernels
- Continuing improvement in NASTRAN based on access to the largest models in the world
- Reduction in CPU time and memory requirements for the sparse solvers
- Demonstration of the value of MSC/NASTRAN for design optimization of large dynamics simulations

These are highlights of the strong partnership between Cray Research and the MacNeal-Schwendler Corporation (MSC). For 15 years, Cray Research has worked with MSC and its popular general purpose finite element analysis program, MSC/NASTRAN.

The goal of our partnership with MSC is to ensure that our mutual customers get the most from each and every new level of performance in MSC/NASTRAN. Cray Research NASTRAN experts write Cray Research versions of some MSC/NASTRAN routines, optimizing them to run best and fastest on Cray Research hardware. They respond to domestic and international customers with advice about the many different parameters and options available in MSC/NASTRAN. Our experts conduct formal and informal benchmarks and demonstration projects, showing customers what needs to be done to run the job on a particular Cray Research system and running models that customers themselves have not been able to run.

A key example of the Cray Research/MSC partnership is the performance improvement seen in the past five years in sparse matrix methods. In 1989 Cray Research and MSC began working together to test and optimize new sparse matrix methods on real customer jobs; 65,536 degrees of freedom (DOF) was the limit at that time. Today, models of up to 1.5 million DOF can be routinely solved on Cray Research systems—30 to 40 times faster than non-sparse methods allow.

MSC/NASTRAN V67.7, available only on Cray Research systems, includes performance improvements directly suggested by Cray Research's Engineering Applications Group. MSC has since incorporated some of these same improvements in V68, the latest release available on a wide variety of hardware platforms.

U E

Cray Research develops software module for plastic injection molding

A revolutionary software module developed by Cray Research guides the plastic molding analysis process and uses third-party analysis programs to drive the simulation. This new technology, which replaces the single-data-point approach, gives engineers easy access to supercomputer power and lets them simulate many possible combinations of the variables used in plastic injection molding simulation problems.

A plastic part was warping excessively during production, causing significant assembly and aesthetic problems. Accepting the manufacturer's challenge to resolve the problem, Cray Research applications experts used the new software module and the MOLDFLOW plastic injection simulation software to simulate the car company's manufacturing process. The entire investigation took approximately 13 hours on a CRAY C90 system in Eagan, Minnesota. After accurately predicting the warpage that was occurring, Cray Research engineers used MOLDFLOW's diagnostic capabilities to identify the specific cause of the problem. The analysts recommended a single change to the manufacturing process, and the problem was solved.

Cars built today contain an average of 700 pounds of synthetic materials. The average price of a plastic mold for automotive parts can run from $50,000 to well over $1,000,000, with tool build and tryout times of many months. Once built, a mold typically undergoes from three to ten molding trials before being declared ready for production. The major U.S. car companies estimate that eliminating just one trial run for a single mold could save as much as $40,000 and six weeks of time.

Cray Research's plastic injection molding team designed Cray Research's new software module to wrap around the molding simulation software modules, take advantage of the power of a supercomputer, and allow for "design of experiments"—running a whole array of variables at once instead of one run at a time.

"As Cray Research has expanded its product line, from the entry-level systems to the highly parallel end, cooperation between MSC's software developers and members of Cray's Engineering Applications Group (EAG) has become even more crucial. This cooperation produced excellent results on our production system of MSC/NASTRAN version 68, which is the best Cray Research version of NASTRAN that we've ever had. Cray's EAG personnel directly suggested some of the performance-related improvements, especially in the I/O area. Other improvements could not have been made without Cray's generous assistance in computing power and computer science support.

"MSC believes in its cooperation with Cray Research, and we are committed to continuing this teamwork in order to provide our joint customers with the best possible software/hardware tool in the Cray Research versions of MSC/NASTRAN."

Dr. Louis Komzsik
Chief Numerical Analyst
MacNeal-Schwendler Corporation

FOC

The Applications Department mission is to help customers achieve their technical and business objectives by providing high-value, high-performance applications solutions. This includes supporting strategic third-party vendors; developing and supporting applications solutions to open new markets; and overcoming computational barriers to industrial productivity through consulting and customer partnerships.

To achieve our mission, we *collaborate* with over 430 software developers to support a broad spectrum of application programs available on Cray Research platforms. We *optimize* Cray Research customers' applications software to ensure they are based on the most current scientific theories and the most efficient mathematical algorithms. We *consult* with users about how to take advantage of Cray Research systems in all three major high-performance computing architectures—the CRAY C90, CRAY Y-MP, large-memory CRAY M90, and CRAY EL90 parallel vector processing supercomputers; the CRAY T3D massively parallel processing system; and the CRAY SUPERSERVER 6400 symmetric multiprocessing system. We *provide* the necessary computer *resources* for customers and developers to test and evaluate high-performance codes for their particular workloads and environments. Our applications laboratory in Eagan, Minnesota, includes a wide variety of state-of-the-art scientific workstations and advanced supercomputing tools linked to Cray Research systems through a worldwide network. We use this lab to provide training, seminars, and demonstrations to customers and prospects. We *conduct* formal and informal *benchmarks*, working side-by-side with customers on real-world problems and "What if?" scenarios. We *collect and disseminate information* about new software products, emerging industry trends, and new applications being ported to Cray Research platforms.

After the install: access to experts

When the Hyundai Motor Company chose a CRAY Y-MP 4E system as its first supercomputer ever, engineers at Hyundai's Advanced Engineering & Research Institute, Ulsan, Korea, gained access to a whole new level of technology. With this access came a need for expert advice on how to make the most of it. From August to December 1993, Hyundai engineers and Cray Research applications experts worked daily in Cray Research's applications laboratory in Eagan, Minnesota, to define and refine how Hyundai could perform the integrated car crash analyses that would be possible now with Hyundai's CRAY Y-MP 4E system. The group agreed on three objectives for the visit: perform a full car integrated frontal crash simulation, teach the Hyundai engineers to use and optimize Cray Research's combustion simulation software package, and advance Hyundai's use of production computational fluid dynamics (CFD) analysis.

Using several of the high-performance computing resources in Cray Research's Corporate Computing and Networks facility, including a fully dedicated large-memory CRAY M90 supercomputer, Cray Research applications analysts demonstrated new techniques for building the most comprehensive model possible: how to fold the airbag, how to include the Hybrid III Dummy (the first human-like and most advanced car-crash dummy), and how to integrate the seat belt into the overall model, for example. Working from an initial model that had an airbag, toe panel, and seat only, and conducting separate analyses for each and every piece, the team added more detail—a seat defined with multiple planes, a windshield crossbar, a steering column, a steering wheel, and, eventually, the entire car. Consulting with Engineering Systems International, developer of the PAM-CRASH code Hyundai uses, the team determined the optimal numerical model for the airbag, installed it in the full car model, and began to answer questions about how the dummy would interact with each new component.

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U S

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Hyundai's order for the CRAY Y-MP 4E system included a license for CRI/*Turbo*Kiva, a powerful software environment that Cray Research designed to help reduce the average two-year period needed to test efficiency and emissions of new engines. CRI/*Turbo*Kiva was initially announced in January 1992, and CRI/*Turbo*Kiva 2.0 was introduced at year-end 1993. The Cray Research applications analysts who led this product's development helped Hyundai's engineers get acquainted with this code in particular and with computational methods for combustion in general. Working with a real production problem for the design of a new Hyundai engine, the analysts first brought in a consultant to prepare two computational grids for the proposed engine. Then the team ran three different problems—steady flow analysis in an intake port, valve, combustion chamber assembly; port fuel injection; and combustion analysis—and prepared video animations of each for the engineers to take back to Korea.

Cray Research has worked with Computational Dynamics Ltd., developer of the CFD program STAR-CD, for two years. When the Hyundai engineers expressed an interest in production CFD analysis, this relationship provided a conduit so that state-of-the-art models from the vendor—porous modeling for radiators and air conditioner condensers, momentum source terms for modeling and operating the engine compartment fan, and new techniques for accurately computing aerodynamic drag coefficients—were made available to the Hyundai engineers, incorporated in the program, and tested during the engineers' stay. The vendor's involvement helped eliminate difficulties as quickly as possible and kept the group moving in the right direction.

"Our long and close working relationship with Cray's Applications Department has been mutually beneficial for LSTC and Cray Research. Cray Research was one of the very first organizations to work with LSTC and our LS-DYNA3D program. The Applications Department has continually delivered exceptional technical and marketing support. Their assistance has helped make LS-DYNA3D one of the most efficient high-performance codes on Cray Research platforms. In addition, Cray's applications specialists continue to demonstrate a genuine commitment to customer support, taking on and successfully completing a number of joint projects between Cray, LSTC, and our mutual customers. As LSTC expands the use of LS-DYNA3D, especially within industry, Cray's applications experience and expertise will continue to be extremely valuable and influential."

Dr. John Hallquist
President and Founder
Livermore Software Technology Corporation

The power of partnership: Bayer AG and Cray Research collaborate on plantwide dynamic process simulations

Challenging production requirements, changing product mixes, and stringent environmental regulations are constants in the worldwide chemical industry. As today's chemical companies grapple with these and other market realities, supercomputer simulation and optimization is a practical tool for improving the economic efficiency, environmental acceptability, quality, and safety of production processes plantwide.

Improved product yield, reduced energy consumption, and enhanced process control and operability were the bottom-line results when Bayer AG and Cray Research teamed up to develop a plantwide dynamic model for a complex, interlinked distillation system. With the SPEEDUP program from Aspen Technology, the model of more than five coupled distillation columns required the repeated solution of a differential-algebraic system with more than 75,000 equations. This is the largest known industrial SPEEDUP application in production use in the world.

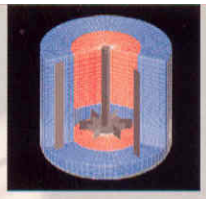
Software optimization and algorithm developments, including a new sparse matrix solver, provided more than a 50-fold increase in SPEEDUP performance. Coupled with the power of a CRAY C90 system, these software enhancements reduced model development time by at least six months compared to workstations and allowed the engineers to obtain fast turnaround times for SPEEDUP input translation and problem solution—a critical requirement for developing plantwide dynamic models for complex industrial processes. The dynamic simulations also provided valuable insight into the placement of plant measurement and control equipment.

Cray Research applications experts support a wide variety of process simulation software from the leading commercial application vendors. ASPEN PLUS and PRO/II are available for steady-state simulation. The SPEEDUP program can be used for dynamic simulation as well as process control, optimization, data reconciliation, and parameter reconciliation. For separation processes, BATCHFRAC for batch distillation and RATEFRAC for rate-based distillation are optimized for Cray Research systems. Other packages include NOVA for large-scale optimization and PIPEPHASE for solving single and two-phase flows through piping networks.

A X P

"The CRAY C90 system and applications support from Cray Research have played a significant role in the development of a powerful time-domain Computational Electromagnetics (CEM) capability at Rockwell Science Center. Today, many large-scale CEM computations can be done routinely and reliably—without system breakdowns or compiler bugs—only on the CRAY C90 system."

Vijaya Shankar
Director, Computational Sciences
Rockwell International Science Center



E R T I S E

Cray Research applications analysts work closely with the Cray Research hardware and software development teams in Chippewa Falls, Wisconsin, and in Eagan. They collaborate with application vendors who develop the most popular high-performance computing solutions. And they work daily to understand the day-to-day objectives customers must accomplish with high-performance computing. This unique set of relationships allows the Applications Department to constantly reevaluate technology, determine how Cray Research hardware and software strategies mesh with current and future customer requirements, and link the latest advances to customers' workplaces.

The Cray Research Applications Department is organized into dedicated application software groups to address the needs of major industries and areas of computational research and product development (below). Working with vendors and customers, these groups have made the Cray Research Applications Department the link between bottom-line business objectives and high-performance solutions.

Value-added applications expertise from Cray Research includes:

Casting
Nuclear engineering
Fluid mixing
Electromagnetics
Process simulation
Grid generation
Database management
Reservoir simulation
Linear programming
Distributed applications
Statistical mechanics
Meteorology
Computational fluid dynamics
Earth sciences
Combustion
Numerical methods
Graphics
Crash simulation
Quantum chemistry
Injection molding
Design optimization
Seismic analysis
Materials science
Electronics
Structural analysis

Cray Research joins international Fluid Mixing Processes consortium

The objective:

To improve the profitability, effectiveness, and safety of fluid mixing in the process industries through an improved understanding of the fluid mechanics involved.

The partners:

- The British Hydromechanics Research Association
- The Fluid Engineering Centre Chemical
- Biochemical manufacturers and process plant operators
- Equipment manufacturers and contractors

The means:

- Long-term collaborative generic research
- Engineering design information and design guides
- Contract research, design, and development
- Consultancy and troubleshooting

In 1994 Cray Research joined this Fluid Mixing Processes (FMP) consortium, an international research, design, and development partnership for the process industries. Cray Research applications experts now collaborate with the world's leading makers and users of the fluid mixing equipment found in process plants across the globe. These partners include, among others: BP Chemicals, Chemineer, Dow Chemical Company, DuPont, Eli Lilly, Kodak, 3M, Merck Sharp and Dohme, Monsanto, Procter and Gamble, Rohm and Haas, and UpJohn Corporation. Together, FMP members tackle subject areas directly related to the needs of FMP members. Past and current projects include:

- Gas/liquid mixing and mass transfer
- Solid suspension and solid/liquid mixing
- Measurement of flow patterns and turbulence by laser doppler anemometry
- Fluid flow and mass transfer in bioreactors and fermentation vessels
- Mechanical loading under steady and transient conditions
- Liquid jet mixing

Empress Software, U.S. Navy, and Cray Research create open systems database

Researchers at the U.S. Navy's Fleet Numerical Meteorology and Oceanography Center (FNMOC) worked with Empress Software and Cray Research's database applications experts to implement a database management system (DBMS)-controlled production and archive database with hundreds of gigabytes of data using Cray Research systems and file servers on a network.

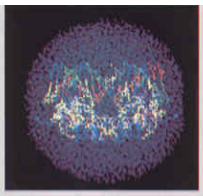
With technical support and computer resources from Cray Research, Empress ported and optimized its EMPRESS relational database management system for Cray Research architecture in a heterogeneous distributed environment. With this system, users may access data transparently from any node on the network and need not know where or how that data is stored. The DBMS also provides concurrency control and added security to ensure data consistency and integrity. FNMOC took advantage of EMPRESS' Binary Large Object (BLOB) capability by writing a library of routines to define their datatypes. This library is called the Integrated Stored Information System (ISIS). Not only does ISIS define specific datatypes for oceanographic and meteorological data such as satellite images, it also allows users to get data in and out of the database without needing to know the Structured Query Language.

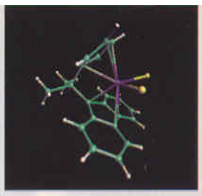
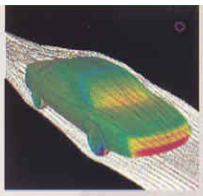
Taking advantage of commercial off-the-shelf software technology saved FNMOC the substantial time required to write software in-house and created an open systems solution using industry standards. Since EMPRESS uses the UNIX file system for storing tables, this software could be used in conjunction with file server technology for managing very large volumes of data.

A N

"Cray Research has helped us improve the performance of our software. Their optimization of the ANSYS program on Cray hardware has led to high levels of performance in parallel processing and I/O, resulting in award-winning performance for ANSYS."

Dr. John A. Swanson
Founder and Chief Technologist
Swanson Analysis Systems, Inc.



S W E R S

In addition to its support of third-party software vendors and their programs, Cray Research has developed some of its own applications. UniChem is an easy-to-use, integrated software environment that incorporates three quantum chemistry methods—ab initio, semi-empirical, and density functional theoretical techniques—into one package with a common user interface. This allows researchers to model and explore, from their desktops, a wide variety of complex molecular systems at a new level of detail. Cray Research developed and enhanced UniChem through a consortium that included Asahi Chemical, E.I. du Pont de Nemours & Co., Eli Lilly and Company, Exxon Research and Engineering, and Sumitomo Chemical. As part of UniChem, Cray Research developed its Application Integration Toolkit to simplify and accelerate the development and use of distributed applications in several ways.

Announced in June 1994, the Cray Research HEXAR application software uses unique, patented algorithms to convert computer-aided design (CAD) surface descriptions of objects into 3-D finite element volume meshes. These meshes, or grids, can contain hundreds of thousands of hexahedral (brick-shaped) elements in typical computational fluid dynamics (CFD) or structural analysis problems. The HEXAR automatic mesh generator product helps engineers avoid the traditional method of hand-crafting these meshes; engineers can explore more design options and build meshes in minutes instead of weeks or months.

CRI/*Turbo*Kiva is a combustion simulation software package designed by Cray Research in collaboration with the Los Alamos National Laboratory to help reduce the average two-year period needed to test efficiency and emissions of new engines. Customers including the Hyundai Motor Company and Nissan use CRI/*Turbo*Kiva to study and optimize fuel injection, intake, ignition, and even two-stroke scavenging.

Dow Chemical Company and Cray Research conduct molecular orbital calculations for plant design

When chemical reactions are involved in a process simulation problem, chemists must provide chemical engineers with important thermodynamic data about the compounds relevant to the simulation. The accurate and most effective design of a chemical plant in which chemical reactions occur depends on knowing the heat of formation—the energy involved in the formation of one mole of a compound from the constituent elements—of the compounds in the plant. Experimental determination of heats of formation, especially for the large, realistic molecular systems found in today's chemical plants, can be too costly and, in some cases, impossible. Here again, state-of-the-art software and the power of Cray Research supercomputers help chemists overcome these barriers.

Accurate ab initio calculations such as the G2 method, though computationally demanding, provide an alternative tool in the quest for heats of formation. Using the *Gaussian 92* program, chemists at the Dow Chemical Company and Cray Research were able to compute heats of formation for several five- and six-membered heterocyclic molecules. All of the calculations were performed on Cray Research supercomputers. These calculations were made practical by taking advantage of Cray Research's supercomputer architecture to efficiently run MP4 and QCISD(T) calculations.

In March 1994 the Dow Chemical Company entered into a three-year collaboration with Cray Research to further advance supercomputing for chemical process engineering. As part of the agreement, Dow has access to a CRAY C92A supercomputer located at Cray Research's computer facility in Eagan, Minnesota. Dow uses the system for chemical process simulation to optimize full plant operations, computational fluid dynamics for chemical mixing simulations in large stirred tanks, and other unit operations commonly used to produce chemical-based products, as well as for computational chemistry and environmental modeling.

For further information,
please contact your Cray
Research representative, or

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Applications images, Page 2, left to right: Cylinder head model with 192,000 degrees of freedom and 2400 RMS wavefront, analyzed with the ABAQUS software package; simulation of metal forming produced with the ABAQUS software package; volume mesh for the fluid and thermal analysis of the engine compartment in a Ford Taurus, courtesy of Ford Motor Company Advanced Vehicle Systems Engineering; stereochemical model of the transition structure for endo trapping of the bicyclo-[2.1.0]pent-2-yl radical by H_2S, calculated with the *Gaussian 92* quantum chemistry program; a MOLDFLOW filling analysis for an automotive intake manifold. **Page 4:** Simulation of an automobile instrument cluster bezel; concentration fields of the transport of two chemical species, shown at various intersections of an inline static mixer's helical mixing elements as the mechanism has passed through various rotations, courtesy of Chemineer, Inc.; MOLDFLOW warpage analysis of a Kia Motors four-cylinder engine intake manifold; finite element model of a human femur, courtesy of Lamb and Company; frontal impact simulation with dummy, courtesy of Kia Motors Corporation. **Page 7:** Space Shuttle Solid Rocket Motor factory joint pressure simulation; image of concentration of fresh charge and velocity streamlines during the scavenging process in a two-stroke engine; chemical mixer vessel modeled with the STAR-CD software, courtesy of Computational Dynamics/adapco; a 10,000-element model of an automotive structural body component; four-cylinder engine block test rig modeled with the STAR-CD software package. **Page 9:** The glucocorticoid receptor interacting with a 17 base-pair nucleotide sequence of DNA, which is contained in an 80 Ångström water droplet, courtesy of Lester Harris, Abbott Northwestern Hospital; a fragment of the Kevlar polymer, approximated with 11 monomeric units; a molecular model of isopropylidene (9-fluorenyl) cyclopentadienyl zirconium dichloride; external airflow over the Dodge Intrepid, modeled with FIDAP; bird strike simulation using LS-DYNA3D, courtesy of Allison Gas Turbine.

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