Collaborations with Industry on Parallel Computing

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The Computational Testbed for Industry (CTI) was established at the Laboratory in 1991 to provide U.S. industry with access to the computing environment at our Advanced Computing Laboratory and to the technical expertise of Los Alamos scientists and engineers. During this past year the CTI was designated officially as a Department of Energy User Facility. That designation affords us greater flexibility in establishing and implementing collaborative agreements with industry. The number of collaborations has been increasing steadily and will soon total about thirty. The seven projects described here are being established at the CTI through the new cooperative agreement between the DOE and Cray Research, Inc. under the auspices of the DOE's High Performance Parallel Processor program. The projects focus on developing scientific and commercial software for massively parallel processing.

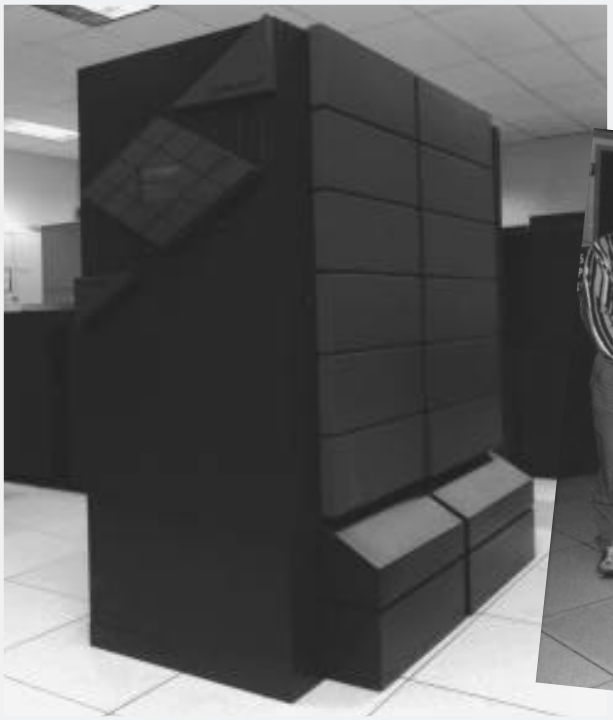
Portability Tools for Massively Parallel Applications Development
Partners: Cray Research, Inc.; Thinking Machines Corporation
Goals: At present, software developed for one vendor's massively parallel computer system is not portable, that is, able to be run on other vendors' computers. The lack of portable programs has slowed the development of applications for every kind of massively parallel computer and the adoption of such computers by industry. This project will work toward removing that barrier by creating common programming conventions for massively parallel machines.

Massively-Parallel-Processing Performance-Measurement and Enhancement Tools
Partner: Cray Research, Inc.
Goals: Create a set of software tools to improve analysis of the system-level performance of massively parallel systems, to maximize their operating efficiency, and enhance the design of future systems. Plans include using this sophisticated automated toolkit to enhance the performance of applications developed in other projects under the cooperative agreement between the Department of Energy and Cray Research, Inc.

Lithology Characterization for Remediation of Underground Pollution
Partner: Schlumberger-Doll Research
Goals: Develop three-dimensional modeling software to cut the costs of characterizing and cleaning up underground environmental contamination. The software is intended for use by the petroleum and environmental industries on the next generation of massively parallel supercomputers.

Development of a General Reservoir Simulation for Massively Parallel Computers
Partners: Amoco Production Company; Cray Research, Inc.
Goals: Oil and gas exploration requires simulations of flow at several million points in reservoirs. Programmers have produced well-developed reservoir simulations for multiprocessor vector supercomputers but not for massively parallel systems, so exploiting the potential of massively parallel computers is a high priority. The goal of this project is to adapt Amoco's field-tested reservoir-simulation software so that it performs efficiently on the massively parallel Cray T3D. The resulting program, which will allow much better management of reservoirs, will be made available to the entire petroleum industry.

Materials Modeling
Partner: Biosym Technologies Incorporated
Goals: In the competitive global marketplace for advanced materials, the traditional experimental approach to designing new materials needs to be complemented by materials modeling using high-performance computers. This project is aimed at creating powerful new visual-modeling software tools to improve casting and welding processes and to calculate the fracture properties of new materials designs, including composites.



At left: The Cray T3D was delivered to our Advanced Computing Laboratory in June 1994. It is a 128-processor machine that will be used primarily for collaborative research with industry. Below: Scientists and engineers from Cray Research, Inc. and Los Alamos at a dedication of the new machine.

Application of the Los Alamos National Laboratory Hydrocode Library (CFDLIB) to Problems in Oil Refining, Waste Remediation, Chemical Manufacturing, and Manufacturing Technology

Partners: Exxon Research and Engineering Company; General Motors Power Train Group; Rocket Research Company; Cray Research, Inc.

Goals: The speed and memory size of massively parallel systems will make it possible for U.S. industry to accurately model and improve the efficiency of chemical reactions that involve substances in more than one phase (solid, liquid, or gas). The project with Exxon will advance the simulation of multiphase reactors, which are heavily used in hydrocarbon refining, chemical manufacturing, gas conversion, and coal liquefaction and conversion. The goal of the General Motors project is to improve analysis of important foundry processes. One of the Rocket Research projects is aimed at improving small electric rockets used in satellite stations and has potential applications to microelectronics manufacturing and to neutralizing wastes in flue-gas emissions. Another Rocket Research project involves analysis of the performance, safety, and environmental impact of propellants used in automotive air bags and in fire-suppression systems of aircraft and other mass-transportation vehicles.

Massively Parallel Implicit Hydrodynamics on Dynamic Unstructured Grids with Applications to Chemically Reacting Flows and Groundwater Pollution Assessment and Remediation

Partners: Berea Incorporated; Cray Research, Inc.

Goals: Develop advanced software models to help U.S. industry better address problems involving combustion, pollution, and the treatment of contaminated groundwater and surface waters. These models could also be applied to designing engines, extracting more oil and gas from fields that have been drilled over, and assessing the structural integrity of buildings after a severe fire.