ENERGY SCIENCE AND TECHNOLOGY SOFTWARE CENTER

Edwin M. Kidd, Director

The Energy Science and Technology Software Center (ESTSC), is the U.S. Department of Energy's (DOE) centralized software management facility. It is operated under contract for the DOE Office of Scientific and Technical Information (OSTI) and is located in Oak Ridge, Tennessee. The ESTSC is authorized by DOE and the U.S. Nuclear Regulatory Commission (NRC) to license and distribute DOE- and NRC-sponsored software developed by national laboratories and other facilities and by contractors of DOE and NRC. ESTSC also has selected software from the Nuclear Energy Agency (NEA) of the Organisation for Economic Cooperation and Development (OECD) through a software exchange agreement that DOE has with the agency.

The ESTSC collection consists of almost 900 software packages ready for distribution, and the Center has several hundred older packages that can be made ready on request. The packages available from the Center are applicable to solving many problems in energy, science, environment, administration, mathematics, and computing. Software packages are primarily applications-oriented and developed to run on personal computers, workstations, mainframes, and supercomputers. Packages are also available where the same source code can be loaded on different types of computers. These are defined as multi-platform and are treated as a fifth platform type in the Center rate structure. The Center with copies of TOUGH for three different platforms (Cray, DEC, and SUN) parallels the multiple-version availability of many of the packages. TOUGH2 for the PC, which will soon be available from ESTSC, is a multi-platform package.

Through an agreement with the Radiation Shielding Information Center (RSIC) at the Oak Ridge National Laboratory, DOE-sponsored, unlimited software that falls within the RSIC scope is announced by the ESTSC but is distributed by RSIC. Software packages and inquiries relating to those packages are forwarded to RSIC. ESTSC is designated by NRC as the primary source for their packages regardless of scope.

The ESTSC has agreements for joint activities with the Computer Software Technology Transfer Center (COSMIC), which distributes software sponsored by the National Aeronautic and Space Administration. These activities include announcements of software availability via a joint newsletter, shared conference exhibits, and a combined catalog on diskette. The agreements also include discounts for sponsoring organizations.

Unlimited software (not copyrighted by the developer) is available for general distribution by ESTSC. Copyrighted software is, in general, made available for government related usage by distribution to DOE, DOE contractors, and other federal agencies. In some cases it may also be distributed to other federal agency contractors.

Requests from organizations wishing to use copyrighted software for nongovernment purposes are referred to the copyright holder except for cases where the copyright holder has approved distribution by ESTSC. Unlimited (noncopyrighted) software is available to the public but is withheld by DOE from foreign dissemination for two years after licensing. Exceptions may be made if the sponsoring DOE office approves the dissemination prior to the end of the two-year withholding period and verifies that U.S. competitiveness will not be adversely impacted by foreign dissemination of the software.

The centralized management of DOE software was done at the National Energy Software Center (NESC), Argonne National Laboratory, from about 1965 until December 1991 at which time the collection was moved to the ESTSC in Oak Ridge. The move of about 2000 packages included TOUGH and the first release of TOUGH2. NESC distributed 27 copies of the software during the time period of 1988 through 1991.

The NESC rights to distribute the Harwell MA28 mathematical routines used in the TOUGH and TOUGH2 packages were in a license that NESC obtained from Harwell. It was determined that the license did not transfer to ESTSC with the move of the software. The distribution of the TOUGH/TOUGH2 software by ESTSC was delayed for a period of time to establish an agreement with Harwell that recognizes the transfer of the rights to ESTSC. From the first part of 1992 until late in 1994, ESTSC has distributed 48 copies of TOUGH and TOUGH2.

Following receipt of the preconditioned conjugate gradient solvers in November 1994 their availability was announced to all recipients of TOUGH and TOUGH2 and distributed to those responding to the announcement. Inquiries are still being received. This distribution of an addendum to a package is a departure from the ESTSC operating policy. The preconditioned conjugate gradient solvers have been added to all ready versions of TOUGH2 offered by ESTSC.

The PC-version of TOUGH2 was received in January 1995 and is expected to be screened and available for distribution before the end of February 1995. Its availability will be announced to all who have made inquiries and to previous recipients of the TOUGH and TOUGH2. This version of TOUGH2 is being offered as a multi-platform code, a platform category now being used by ESTSC for several packages.

Primary Center functions include software package receipt, review, screening, and in some cases testing; responding to inquiries and orders received via phone, fax, mail, and E-mail; dissemination of general Center information, specific package information, and software packages; and reporting to the agencies on overall Center operation. Other Center functions include interfacing with the agencies on operating

and policy questions and with Center partners on various agreements; working with package developers to resolve questions relating to submitted or requested packages; and announcing and exhibiting the Center software.

DOE expects the ESTSC to recover from package fees all operating costs related to processing DOE-sponsored packages. NRC supports part of the cost relating to Center processing of their packages and expects the balance to be recovered from fees charged for the packages. As DOE-sponsored software, processing costs related to TOUGH and TOUGH2 are to be recovered from fees charged for package distributions.

Pricing of software packages is determined on the basis of customer category: DOE (includes DOE offices, DOE contractors, other Federal agencies, U.S. educational institutions, and Cooperative Agreement Partners), public, or foreign. Platforms include personal computers (PC), workstations (WS), mainframes (MF), supercomputers (S), and multi-platform (MP).

Customer Category	PC	WS	MF	S	MP
DOE	$ 250	$ 400	$ 500	$ 1,200	$ 600
PUBLIC	510	1,305	1,835	4,560	2,200
FOREIGN	940	2,000	2,715	6,700	3,300

General information items available on request include a brochure (ESTSC-B1) that contains general information about the Center, the ESTSC Software Listing (ESTSC-2/Rev.3) that provides a listing and brief description of software packages in paper copy, and a joint ESTSC/COSMIC catalog on diskette. Internet users can access the file through the DOE Home Page as shown below and can contact ESTSC via E-mail or other methods as listed below.

U.S. Mail:	Energy Science and Technology Software Center P.O. Box 1020 Oak Ridge, TN 37831-1020
Commercial Carrier:	175 Oak Ridge Turnpike Oak Ridge, TN 37830
Phone:	615/576-2606
Fax:	615/576-2865
Internet E-mail:	estsc@adonis.osti.gov

World Wide Web (WWW) server: Use one of the following Uniform Resource Locators.

http://www.doe.gov

Accesses the DOE Home Page.

http://www.doe.gov/html/osti/estsc/estsc.html

Accesses general ESTSC information including the software catalog.

http://www.doe.gov/waisgate/estsc.html

Accesses the ESTSC software catalog.