Applied Mathematical Sciences

Applied Mathematical Sciences research aims at advancing knowledge of mathematical and computer sciences and computing techniques related to energy research, production, and distribution. It also manages high performance supercomputing facilities.

EISPACK AND LINPACK

Reinventing the wheel is generally recognized as a waste of time. But, for many years, a practice much like reinventing the wheel was the order of the day in scientific and engineering computation. Engineers or scientists seeking to solve commonly encountered mathematical equations had to write their own computer programs to perform the necessary calculations.

EISPACK and LINPACK, two pioneering collections of subprograms created by a team of Argonne National Laboratory and university researchers, ended much of this waste. Engineers and scientists could solve commonly encountered mathematical problems by simply calling on these "canned" subprograms. Thus, this accomplishment significantly increased productivity in a number of different fields—from electronics to structure analysis to molecular physics. Not only have these pacesetting packages been widely used themselves, but they have become standards of excellence against which other mathematical software is compared.

The use of mathematics in all fields of science, engineering, and economics naturally divides into two parts. The first part involves the construction of a theoretical or engineering mathematical model for the phenomena being investigated, that is,.setting up the equations to be solved. The second part involves solving the equations. If that requires finding **eigenvectors** and **eigenvalues** of a mathematical operator, EISPACK can be used. If the model involves the solution of a system of linear equations, LINPACK is called for. The scientist or engineer can use EISPACK and LINPACK with confidence that computations will be done accurately and efficiently, and he or she can concentrate on parts of the problem requiring creative thought.

EISPACK is a contraction for "Eigensystem Package." EISPACK routines are used to solve what is known in the mathematical literature as a **matrix eigensystem problem**. Matrix eigensystem problems are encountered in many otherwise unrelated fields. They appear, for example, in studies of molecules, atoms, and the fundamental constituents of matter. They also appear in investigations of natural modes of vibration, whether the vibrations of interest are the swaying of a bridge or steel-framed building, the flutter of an airplane's wings or airframe, or the transient oscillations of an electrical network or electromechanical device. Some problems require computation of quantities called **eigenvalues** and **eigenvectors**, which together comprise an **eigensystem**.

In the physics and chemistry of molecules, atoms, and fundamental particles, each eigenvalue corresponds to one of the energy levels of a molecule, atom, or particle. Together with its eigenvector, each eigenvalue gives information about the form of matter that is present, its energy level, and its readiness or suitability to be involved in a reaction or interaction.

In mechanical systems such as an airplane wing or automobile suspension, each eigenvalue corresponds to one of the vibration frequencies that occur. Each eigenvector identifies the shape of the vibrating structure and magnitude of the vibration associated with one specific frequency. The first eigensystem corresponds to the base or fundamental frequency, the second to the first overtone or harmonic that is present, and so forth.

Solving matrix eigensystem problems is one of the most challenging tasks faced by scientists and engineers. Thus, it is one of the few areas where mathematical purists **do not** recommend avoiding