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Tools for scientific computation. (English) Zbl 0798.65095

Z. Angew. Math. Mech. 73, No. 12, 335-348 (1993).

Scientific Computation (short: SC) denotes the use of computers for the modelling and simulation of complex scientific and technological processes. Its goal is to perform specified computer simulation related tasks more reliably, quickly and cheaply, and more conveniently for the user. Thus the concept of tools is at the center of SC; the paper attempts a survey of the (1992) status of such tools. It begins with classifications from various points of views; then a number of typical tools are discussed in more detail. (Hardware oriented tools are omitted here.)

As an example of an integrated problem solving environment, //ELLPACK ("Parallel" ELLPACK) is presented and some of its principal aspects are discussed. The remainder of the paper is devoted to a closer look at a few important and novel tools for SC which are not as perfectly integrated as //ELLPACK. It begins with a description of the main features of LAPACK, the (then) new linear algebra library for high-performance computers. As an example of an algebraic tool, the use of Gröbner bases for the computation of zeros of multivariate polynomial systems is described. Tools for "Automatic differentiation" permit the use of analytic procedures in SC. More and more important are automatic restructuring tools which adapt programs to particular concurrent computer architectures. The selection of appropriate codes from program libraries requires yet another type of SC tools.

Some considerations about future developments and a list of relevant journals conclude the article.

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MSC:

65Nxx	Numerical methods for partial differential equations, boundary value problems
65Fxx	Numerical linear algebra
68W30	Symbolic computation and algebraic computation
65Y05	Parallel numerical computation
68-02	Research exposition (monographs, survey articles) pertaining to computer science
65H10	Numerical computation of solutions to systems of equations
13P10	Gröbner bases; other bases for ideals and modules (e.g., Janet and border bases)
35J05	Laplace operator, Helmholtz equation (reduced wave equation), Poisson equation
35J25	Boundary value problems for second-order elliptic equations

Keywords:

software tools; research survey; scientific computation; parallel ELLPACK; automatic differentiation; computer simulation; LAPACK; linear algebra library; high-performance computers; Gröbner bases; zeros of multivariate polynomial systems

Software:

ADIFOR; LINPACK; LAPACK; ELLPACK; EISPACK

Full Text: DOI

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