A numerical, self-consistent field, multi-configuration Hartree-Fock program is described for determining radial wave functions for bound states of atoms and ions. Along with the total energy, the program predicts a number of atomic properties such as the electron density at the nucleus, the mean radius for an electron, values of Slater integrals, and spin-orbit parameter. [The *SCI®* indicates that this paper has been cited in over 185 publications.]

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February 25, 1987

As a mathematics student seeking summer employment, I was always given a computational task using desk calculators. Accepting that role but wishing to compute "first-class," I decided to study computers at Cambridge University. In 1954 Douglas R. Hartree assigned me the problem of solving the "equations with exchange," now known as the Hartree-Fock equations. In those days, programs were written in machine language. I started by writing programs for the EDSAC I, two years later rewrote them for FERUT, and a year later for the ALWAC. Then, in the summer of 1962, while at the Boeing Airplane Company, I was introduced to FORTRAN. I immediately recognized that FORTRAN presented an opportunity for portability between machines and started to work on a multiconfiguration Hartree-Fock (MCHF) program using the self-consistent field method. The following year Margaret Lewis introduced me to David Layzer at the Harvard College Observatory, who provided me with access to the IBM 7090 for several years. During this time the MCHF program and the associated numerical procedures were developed.

Publication of the paper describing this work was made possible through the efforts of Phil Burke, who established the *Computer Physics Communications* journal. It was one of the first to publish descriptions of refereed programs. Prior to 1969 it was only possible to publish the numerical procedures. Such a paper had already been recommended for publication on condition that the problem be an important one! Words to that effect had to be added to the manuscript.

Programs in the public domain often are not cited when used in research, so why was this one? I believe the program was accepted because of its portability and relative ease of use. Citations resulted from the fact that many researchers were able to get on with their science without concern for numerical methods and extensive programming. This has been gratifying since, even as late as 1975, a National Science Foundation (NSF) program director told me NSF did not fund program development and that physicists did not use other people's programs: they wrote their own. A program encapsulating knowledge about the solution of a problem may be a greater research contribution than a paper describing only the procedures. My citations support that view. [For a recent paper on this subject, see reference 1.]

1. Froese Fischer C. Self-consistent-field (SCF) and multiconfiguration (MC) Hartree-Fock (HF) methods in atomic calculations: numerical integration approaches. *Comput. Phys. Rep.* 3:273-326, 1986.