May 15, 2015, Revisited with Source Code Translation and Revision

Back in the May of 2015, I was working on a C# translation of the FORTRAN source code found in the paper:

An adaptive algorithm for numerical integration over an n-dimensional cube - ScienceDirect

Here is my Microsoft TechNet description of my submitted source code:

Multiple integration by means of repeated integration or product formulas possesses what is called the curse of dimensionality which means the number of function evaluations increases exponentially with increasing dimensions. This program implements ***ALGORITHM 006*** *from the excellent paper by Paul van Dooren and Luc de Ridder to be found in the* ***Journal of Computational and Applied Mathematics****, volume 2, no. 3, 1976, pages 207-217. The title of the treatise is "An Adaptive Algorithm for Numerical Integration over an n-Dimensional Cube". I merely translated the FORTRAN IV spaghetti code almost directly from the original to C# via the not so judicious use of switch statements to simulate conditional and unconditional branching statements ("go to" statements in FORTRAN IV). Due to a lack of inclination and time I pretty much adhered to a strict translation of the code. GO TO statements are the bane of structured programming, but once upon a time these branching statements were necessary to early languages like BASIC and FORTRAN. But along came ALGOL 60, ALGOL-W, and Pascal and thus we programmers were rocketed into the pleasant universe of structured programming. The vestige of the "go to" statement is still found in some form in the modern procedural language, C, and its object-oriented offspring C++ and C#.*

I modified my translation to numerically by brute force to compute Coulomb integrals for the helium-like atom. Rather than using a smart method that uses only double integrals I calculated six iterative integrals. The intelligent methodology can be found in the first three references of the References below:

References

[1] L. I. Schiff, Quantum Mechanics Third Edition, New York: McGraw-Hill Book Company, 1968.

[2] I. N. Levine, Quantum Chemistry 2nd Edition, Boston: Allyn and Bacon Inc, 1974.

[3] J. D. Jackson, Classical Electrodynamics Second Edition, New York: John Wiley & Sons, 1975.

[4] H. T. Lau, A Numerical Library in C for Scientists and Engineers, Boca Raton: CRC Press, 1995.

[5] S. D. Conte and C. de Boor, Elementary Numerical Analysis An Algorithmic Approach Third Edition, New York: McGraw-Hill Book Company, 1980.

Here are a couple of results, namely, <1s1s|1/r_12|1s1s> and <1s2s|r_12|1s2s> for Z= 2 helium:

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desired relative error 1e-08:
f#      integral        epsilon         number  err code
1       +1.266501e+00   1.783557e-01    257     0
2       +1.135232e+01   3.351699e+00    257     0
f#      abs error       percent error
1       +1.650092e-02   +1.320074e+00
2       +6.341303e-02   +5.554880e-01
```

For the actual values of the integrals above see the references or for <1s2s|1/r_12|1s2s> see:

Evaluation of the Coulomb and exchange integrals for higher excited states of helium atom, by taken into account the interaction between magnetic moments of the electrons (arxiv.org)