May 3, 1988

An Exercise in Technical Support for Scientific Computation for a Lecture Course presented at SUN Microsystems by Prof. W. Kahan, Univ. of Calif. at Berkeley

Floating-point computation is beset by truths, half-truths and mistakes to an extent little appreciated by the world at large, as this exercise will illustrate. Imagine that you work for CRAY providing technical support for its salesmen and customers, and you have been passed the following letter. This letter is based upon actual events embellished only slightly for didactic effect.

Dear xxxx,

The Fortran function AMOD in both the CFT and CFT77 compilers on a CRAY can give wrong results for certain arguments. Here is an example: PROGRAM:

format(2z16)
format(3z18)
format(....)

format(....)

read 1, x

read 1, y

r = amod(x, y)

print 4, "x", "y", "r"

print 2, x, y, r

print 3, x, y, r

end

INPUT:

4009f9fffffffff 4009fa0000000000

OUTPUT:

x y r 4009F9FFFFFFFF 4009FA000000000 BDFA80000000000 499.999999999818 500.0000000000000 -1.8189894035458565e-12

This violates the definition of AMOD(x, y) = x - AINT(x/y)*y, because when x and y satisfy 0 < x < y, as they do here, then AMOD(x, y) should give a positive number x instead of the negative number x - y. This violation crashed a long benchmark code that had worked perfectly well on an IBM 3090, DEC VAX and SUN III. The code calculates f(x,y) = SQRT(AMOD(x,y))*EXP(-x) among other things for innocuous values x and y that are always positive.

The CRAY has very peculiar division; 240.0/3.0 does not give exactly 80.0 and x/y above yields 1.0 exactly instead of 0.99999... as on all other computers and calculators that I have tried. I can tolerate small errors in quotients, but negative values for AMOD(positive, positive) is too bizarre to tolerate in an environment where we must share standard Fortran codes that run unexceptionably on all our other machines. Negative values cannot occur on the IBM machines because they chop quotients, so AINT(x/y) cannot be wrong. The SUN III conforms to the IEEE standard 754, which prescribes an exact remainder, so it cannot malfunction. The DEC VAX has an EMOD instruction in its architecture, which may explain why its AMOD is always correct.

The CRAY is the odd man out here; if you can't fix it, we don't want it.

Yours

Discussion of

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The allegations about the CRAY's peculiar division are correct as of this date; almost all other computers and calculators do always deliver a quotient x/y < 1 despite roundoff whenever 0 < x < y, so they can guarantee that AMOD(x,y) = x exactly in this case. Indeed, on almost all machines with binary floating-point, AMOD(x,y) is just fine so long as x lies between 0 and about 2.9797*y; on non-binary machines, between 0 and about 1.9997*y. After that, what happens is not easy to predict.

The trouble starts with the definition of AMOD(x,y). Ideally, this is the remainder r you would get after you carried out long division (as you learned it in school) to compute x/y, but stopped as soon as all the digits of the quotient n that precede the decimal point had been generated. Then r = x - n*y where $0 \le r/y \le 1$ and the quotient n is the integer nearest x/y on the same side as zero; n would equal AINT(x/y) in the absence of roundoff. Ideally r can be computed and represented exactly (unless it underflows, but let's skip that for now) in the same floating-point format as x and y provided all the digits of n are generated correctly; that is a challenge because there can be so many of them when |x/y| is very big, so many that most must be rounded away by AINT(n) to fit into the same floating-point format. Now you see where the trouble begins; the definition AMOD(x, y) = x - AINT(x/y)*y

could mean the ideal remainder r, or it could mean the result of computing the rounded values x/y, AINT(x/y), AINT(x/y)*y and x = AINT(x/y)*y in turn. Which is the correct AMOD?

Originally, when Fortran was young, all computers computed the version of AMOD contaminated by a few rounding errors; CRAYs still do it that way and they are not alone. Unfortunately, the contaminated AMOD(x,y) can fail to lie where most users expect it, namely between 0 and y. Only if AINT(x/y) is computed too big in magnitude, as could happen on machines like DEC VAXs that round quotients correctly, can AMOD have the wrong sign; but that cannot happen on machines that chop quotients as did all the old IBM 7094s, the old CDC 6400 and 6600 (but not 7600) and many others machines, and as do all IBM 370's and Amdahls nowadays. Perhaps that explains why the wrong sign for AMOD is such a surprise for old-timers and their programs. On the other hand, a contaminated AMOD(x,y) can easily be bigger than y, but not likely by so much as would be obvious.

All machines that conform to IEEE 754/854 should be able to derive an ideal AMOD quickly from the standards' mandatory remainder operation. Machines that lack a hardware remainder can compute it in software like that supplied in the C Math library distributed with 4.3 BSD Berkeley UNIX. Similar but proprietary software resides in DEC's VAX VMS Fortran library; it doesn't use an EMOD instruction, which is a peculiar multiply.

What should CRAY do? CRAY's floating-point hardware is too inaccurate to support an ideal AMOD at a tolerable cost. The least intrusive alternative may be a loop to test AMOD(x,y) for the correct sign (the same as y's), although only rarely will that test have to correct AMOD (by adding y to it). W. K.