## Additional Content for Use with Classical Fortran

The section numbers in this table show approximately where each addition will go if it is ever included in a Third Edition of the book; + means "between this section and the next at its level, adjusting subsequent section numbers to make room."

| new § | title | contents |
| :--- | :--- | :--- |
| $6.6 .1+$ | Real-to-Integer Functions | truncating and rounding real values to integer |
| $9.6+$ | Undoing End-of-File | appending to a file; reattaching the keyboard |
| $18.4+$ | Extra-Precision Accumulation | computing $\mathbf{x}^{\top} \mathbf{y}$ more precisely |
| $18.5+$ | Generating Pseudorandom Numbers | a generalized shift register algorithm |

### 6.6.1+ Real-to-Integer Functions

I described in $\S 4.4$ how IFIX can be used to find the integer closest to a positive real value (top panel on next page). Often it is necessary to find the integer that is related to a real value in one of the slightly different ways illustrated below. Modern Fortran has built-in functions for ceiling and floor (see §17.1.3) and for the integer nearest a real value.

$\mathrm{K}=\operatorname{ICEIL}(\mathrm{X})=$ lowest integer not less than X
FUNCTION ICEIL(X)
REAL*8 X
ICEIL=IFIX (SNGL (X) )
IF (DFLOAT (ICEIL).LT.X) ICEIL=ICEIL+1
RETURN
END

$\mathrm{K}=\operatorname{IFIX}(\operatorname{SNGL}(\mathrm{X}))=$ truncate fractional part

$\mathrm{K}=\operatorname{IFLOR}(\mathrm{X})=$ highest integer not more than X
FUNCTION IFLOR(X)
REAL*8 X
IFLOR=IFIX (SNGL(X))
IF (DFLOAT (IFLOR). GT.X) IFLOR=IFLOR-1
RETURN
END

$\mathrm{K}=\operatorname{IFIX}(\operatorname{SNGL}(\mathrm{X})+0.5)=$ round positive values

$\mathrm{K}=\operatorname{IROUND}(\mathrm{X})=$ integer closest to X
FUNCTION IROUND (X)
REAL*8 X
IF (R.GT.O.DO) THEN
$\operatorname{IROUND}=\operatorname{IFIX}(\operatorname{SNGL}(R)+0.5)$
ELSE
IROUND $=\operatorname{IFIX}(\operatorname{SNGL}(R)-0.5)$
ENDIF
RETURN
END

$\mathrm{K}=\operatorname{IFIX}(\operatorname{SNGL}(\mathrm{X})-0.5)=$ round negative values

Copyright (c) 2024 Michael Kupferschmid, all rights reserved.
This supplementary textbook Section is licensed under CC-BY 4.0.
Anyone who complies with the terms specified in
https://creativecommons.org/licenses/by/4.0/legalcode.txt
may use the work in the ways therein permitted.

## 9.6+ Undoing End-of-File

When READ sees a *D or encounters the end of a disk file, the I/O library marks that condition by setting a flag. This Section discusses two unusual situations in which persistence of that flag is inconvenient, and shows ways in which it can be reset.

Appending to a file. Some I/O library implementations provide one of these options

```
OPEN(UNIT=unit, FILE=file, POSITION='APPEND')
OPEN(UNIT=unit, FILE=file, ACCESS='APPEND')
```

for positioning the line pointer at the end of a file. If neither option is supported, I suggested in $\S 9.6 .0$ reading the file until its end is reached and then writing more lines to it. That approach fails in implementations, including gfortran, that do not permit the file to be written to or read from after the end-of-file flag has been set. In that case we can resort to the strategy embodied in the APPEND routine listed below.

```
    SUBROUTINE APPEND(NUNIT)
    This routine positions the line pointer at the end of the file
    attached to unit NUNIT so that it can be appended to, without
    leaving the file closed so that it cannot be written.
    variable meaning
    I index on the lines in the file
    LNUM number of line just read
    NUNIT number of logical I/O unit attached to the file
C
C
C count the lines in the file
    REWIND (UNIT=NUNIT)
    LNUM=0
    2 READ(NUNIT,*,END=1)
    LNUM=LNUM+1
    GO TO 2
C
    reread those lines without setting the EOF flag
    1 REWIND(UNIT=NUNIT)
    DO 3 I=1,LNUM
            READ(NUNIT , *)
        3 CONTINUE
        RETURN
        END
```

This routine $14-19$ reads the file once to its end, counting its lines. Then 21-25 it reads that number of lines from the file again, stopping before the end-of-file flag is set. This positions the line pointer to the next line after those already present, so that more lines can be written into the file.

Reattaching unit 5 to the keyboard. Recall from $\S 9.1$ that logical unit number 5 is attached by default to the keyboard, which Unix refers to by a device name such as
/dev/pts/0. Sometimes it is desirable to take the END= exit from READ when an interactive user enters ${ }^{\wedge} D$, perform some action, and eventually resume reading input from the keyboard. After the ${ }^{\wedge} \mathrm{D}$ is received standard-in remains attached to the device, but if the end-of-file flag is persistent attempts to read from the keyboard elicit a Fortran runtime error message such as Sequential READ not allowed after EOF. To re-enable unit 5 for input from the keyboard after doing whatever is appropriate in response to the end-of-file, it is necessary to close and reopen the unit. The UNCTLD routine listed on the next page finds the device name of the keyboard, closes the unit, and reopens it on that device.

The code begins 29 by using INQUIRE to find the name of the file or device that is attached to unit 5 .

If $30-34$ the name begins with the string stdin then unit 5 is reading from a redirection (see $\S 9.4$ ) or a Unix pipe (see $\S 14.1 .0$ ), in which case the end-of-file cannot be rescinded; the routine closes the unit and returns with $R C=3$.

If $36-40$ the name is blank then the unit is already closed. We have no way of knowing what it had been attached to, so the routine returns with $R C=2$.

If 41-46 the name does not begin with the string / dev/ then unit 5 is attached to a file rather than to the keyboard, and in this situation also the end-of-file cannot be rescinded; the routine closes the unit and returns with $R C=1$.

Otherwise 49-52 the routine assumes that unit 5 is attached to the keyboard, so it can clear the end-of-file flag by closing the unit and reopening it on the device to which it was previously attached. To signal this normal outcome the routine returns $\mathrm{RC}=0$.

[^0]```
    1 C
    SUBROUTINE UNCTLD(RC)
    C This routine reestablishes unit 5 as the keyboard after EOF.
    4 C
    5 C RC meaning
    C -- -------
    7 C O all went well; unit 5 was closed and reopened
    8 C 1 unit 5 was attached to a file; unit 5 was closed
    9 C 2 unit 5 was already closed; nothing was done
    unit 5 was a redirect or pipe target; unit 5 was closed
    variable meaning
    FYLE the file or device name to which unit 5 is attached
    NAM the first 5 characters of FYLE
    RC return code; see table above
    formal parameter
        INTEGER*4 RC
        overlay to extract the first 5 characters of FYLE
        CHARACTER*24 FYLE
        CHARACTER*5 NAM
        EQUIVALENCE(FYLE,NAM)
C
C
C
C where is unit 5 attached now?
        INQUIRE(UNIT=5,NAME=FYLE)
        IF(NAM.EQ.'stdin') THEN
            unit 5 is the target of a redirect or pipe
            CLOSE(5)
            RC=3
            RETURN
        ENDIF
        IF(NAM.EQ.' ') THEN
            unit 5 is closed
            RC=2
            RETURN
        ENDIF
        IF(NAM.NE.'/dev/') THEN
            unit 5 is attached to a file
            CLOSE(5)
            RC=1
            RETURN
        ENDIF
        unit 5 is attached to some /dev, presumably the keyboard
        CLOSE(5)
        OPEN(UNIT=5,FILE=FYLE)
        RC=0
        RETURN
        END
```


## 18.4+ Extra-Precision Accumulation

A fundamental operation in numerical linear algebra, first mentioned in $\S 6.3$, is finding the dot product of two vectors $\mathbf{x}$ and $\mathbf{y}$ as the following sum.

$$
\mathbf{x}^{\top} \mathbf{y}=\sum_{j=1}^{n} x_{j} y_{j} .
$$

This calculation is likely to be imprecise because of rounding error in the multiplications and cancellation error when small terms are added into a large sum, as discussed in §4.3. I mentioned there that cancellation error can be reduced by adding up the terms in ascending order of absolute value, but that is seldom done in finding the dot product because precomputing and sorting the products $x_{j} y_{j}$ uses significant extra memory and CPU time. Nonetheless we often want a precise answer, so it is standard practice to instead accumulate the sum at extra precision. For example, if the basic calculation uses REAL*4 numbers the dot product might be coded using REAL*8 arithmetic like this.

```
REAL*4 X(100),Y(100),DOT
REAL*8 Z
:
Z=0.D0
DO 1 J=1,100
    Z=Z+DBLE(X(J))*DBLE(Y(J))
1 CONTINUE
DOT=SNGL(Z)
```

Here the DBLE function (see $\S 4.4$ ) is used to cast $X(J)$ and $Y(J)$ to REAL*8 for the multiplication, and SNGL is used to convert the result Z back to REAL*4. If your compiler supports the REAL*16 data type, you can modify this code to compute accurate REAL*8 dot products. But what if your compiler does not recognize REAL*16, or it does but the basic calculation already uses REAL*16 and you want more precision than that? There is in fact a clever way (see [201], $[202 \S 4.4]$, and $[9, \S 4.3 .3]$ ) to perform the dot product calculation at extra precision with variables of the same precision as those used to store the vectors, and with only a small penalty in memory and processor time.

Multiplying two $n$-bit binary fractions $a$ and $b$ yields a product $a b$ that is $2 n$ bits long, as in this example with $n=4$.

$$
\begin{aligned}
& \text { - } 1110=a \\
& \times \frac{.1101}{1110}=b \\
& 0000 \\
& 1110 \\
& 1110 \\
& \overline{-10110110}=a b
\end{aligned}
$$

To store this result as a 4 -bit binary fraction we must discard the least-significant 4 of its fraction bits, or half of the bits that make up the answer! These bits are of course much less important than the ones we keep, but neglecting them does introduce some error. The right answer is $.10110110_{2}=\frac{1}{2}+\frac{1}{8}+\frac{1}{16}+\frac{1}{64}+\frac{1}{128}=0.7109375_{10}$ but the result we keep is $.1011_{2}=0.6875_{10}$.

Instead suppose we split $a$ into two parts so that $a=a_{h}+a_{t}$, where $a_{h}$ is the value of the high or most-significant $n / 2$ bit positions of $a$ and $a_{t}$ is the value of the trailing or least-significant $n / 2$ bit positions. Then, if $a_{h}$ and $a_{t}$ are stored as floating-point binary fractions having $n$ significand bits, the rightmost $n / 2$ bits in each of them will be zero. Splitting $b$ will yield parts $b_{h}$ and $b_{t}$ that similarly have zeros in their $n / 2$ least-significant bit positions. Then we can find the product as

$$
a b=\left(a_{h}+a_{t}\right)\left(b_{h}+b_{t}\right)=a_{h} b_{h}+a_{h} b_{t}+a_{t} b_{h}+a_{t} b_{t}
$$

where each partial product is exactly represented by a floating-point binary fraction of $n$ bits and can therefore be stored without any loss of precision. For our $n=4$ example this is how the process works.

$$
\begin{aligned}
a & =.1110=.1100 \times 2^{0}+.1000 \times 2^{-2}=a_{h}+a_{t} \\
b & =.1101=.1100 \times 2^{0}+.0100 \times 2^{-2}=b_{h}+b_{t} \\
a_{h} b_{h} & =\left(.1100 \times 2^{0}\right) \times\left(.1100 \times 2^{0}\right)=.1001 \times 2^{0} \\
a_{h} b_{t} & =\left(.1100 \times 2^{0}\right) \times\left(.0100 \times 2^{-2}\right)=.0011 \times 2^{-2} \\
a_{t} b_{h} & =\left(.1000 \times 2^{-2}\right) \times\left(.1100 \times 2^{0}\right)=.0110 \times 2^{-2} \\
a_{t} b_{t} & =\left(.1000 \times 2^{-2}\right) \times\left(.0100 \times 2^{-2}\right)=.0010 \times 2^{-4}
\end{aligned}
$$

Each of the parts has $n / 2=2$ trailing zeros, and each partial product just fits in $n=4$ bits. If we align binary points and add partial products we get the same answer as before.

$$
\begin{aligned}
& .10010000=a_{h} b_{h} \\
& .00001100=a_{h} b_{t} \\
& .00011000=a_{t} b_{h} \\
& .00000010=a_{t} b_{t} \\
& . .10110110=a b
\end{aligned}
$$

To avoid losing the least-significant half of this result, we could accumulate the sum of the partial products into a two-element vector of 4 -bit floating-point binary fractions, ending up with $a b=\left[\left(.1011 \times 2^{0}\right),\left(.0110 \times 2^{-4}\right)\right]$. Once a whole dot product has been accumulated, the less-significant parts of all the partial products will have added up instead of being lost through cancellation, and we can obtain an accurate $n$-bit answer by adding the two $n$-bit vector elements that we used to store the $2 n$-bit sum.

The MPYACC subroutine listed on the next page uses the splitting idea to perform a single multiplication of the scalar X times the scalar Y, calling ADDACC to add each partial product to the two-element accumulator XYSUM. Unlike $a$ and $b$ in the discussion above, X and Y are 21 REAL*8 variables. According to $\S 4.2$ they have a sign bit and 11 exponent bits preceding an implied " 1 ." and 52 bits of binary fraction, so in splitting them it is necessary to preserve the sign and exponent bits. To split $X$ we begin 35 by copying it into XH , which is 25-26 overlaid by the two-element INTEGER*4 vector IXH. On a little-endian processor the least-significant word of $X$ comes first in memory (see §4.8) so another name for it is IXH (1). This fullword we bitwise-AND (see $\S 4.6 .3$ ) with HMASK 37 which is initialized 27 at compile time to the bit pattern 1111110000000000000000000000000 . The resulting value of XH is thus X with its least-significant $26(=n / 2$ in the discussion above) bits set to zero. We want XH and XT to add up to X , so 38 XT is just X minus the XH we found. The same process is used $39-42$ to split Y into YH and YT. The parts XH, XT, YH, and YT, are REAL*8 so they have 52 fraction bits, but of these the trailing 26 are zero. Finally the code 45-52 computes the four 52 -bit partial products (in order from smallest to largest) and adds each to the extra-precision accumulator.

| 1 |  | SUBROUTINE MPYACC (X,Y, XYSUM ) |
| :---: | :---: | :---: |
| 2 |  | This routine accumulates XYSUM=XYSUM $+\mathrm{X} * Y$ at extra precision. |
| 3 |  |  |
| 4 |  | variable meaning |
| 5 |  | -------- ------- |
| 6 | C | ADDACC routine adds to an extra-precision accumulator |
| 7 | C | HMASK deletes the 26 least-significant fraction bits |
| 8 |  | IAND Fortran function for bitwise logical AND |
| 9 | C | IXH XH as 2 fullwords |
| 10 | C | IYH YH as 2 fullwords |
| 11 | C | P a partial product |
| 12 | C | X first number in product |
| 13 | C | XH split of X containing its high 26 fraction bits |
| 14 | C | XT split of $X$ containing value of trailing 26 bits |
| 15 | C | XYSUM extra-precision accumulator |
| 16 | C | $Y$ second number in product |
| 17 | C | YH split of Y containing its high 26 fraction bits |
| 18 | C | YT split of Y containing value of trailing 26 bits |
| 19 | C |  |
| 20 | C | formal parameters |
| 21 |  | REAL*8 X,Y,XYSUM(2) |
| 22 | C |  |
| 23 | C | prepare to split X and Y |
| 24 |  | REAL*8 XH, XT, YH, YT |
| 25 |  | INTEGER*4 IXH(2), IYH(2) |
| 26 |  | EQUIVALENCE (XH, IXH) , (YH, IYH) |
| 27 |  | INTEGER*4 HMASK/Z'FC000000'/ |
| 28 | C |  |
| 29 | C | prepare to compute the partial products |
| 30 |  | REAL*8 P |
| 31 | C |  |
| 32 | C |  |
| 33 | C |  |
| 34 | C | split X and Y into parts having 26 trailing fraction bits zero |
| 35 |  | XH=X |
| 36 | C | this assumes the processor is little-endian |
| 37 |  | $\operatorname{IXH}(1)=\operatorname{IAND}(\operatorname{IXH}$ (1) , HMASK) |
| 38 |  | XT=X-XH |
| 39 |  | YH=Y |
| 40 | C | this assumes the processor is little-endian |
| 41 |  | IYH (1) $=\operatorname{IAND}$ ( $\mathrm{IYH}(1)$, HMASK ) |
| 42 |  | $\mathrm{YT}=\mathrm{Y}-\mathrm{YH}$ |
| 43 | C |  |
| 44 | C | add the 52-fraction-bit exact partial products to accumulator |
| 45 |  | $\mathrm{P}=\mathrm{XT} * \mathrm{YT}$ |
| 46 |  | CALL ADDACC (P,XYSUM) |
| 47 |  | $\mathrm{P}=\mathrm{XT} * \mathrm{YH}$ |
| 48 |  | CALL ADDACC (P, XYSUM) |
| 49 |  | $\mathrm{P}=\mathrm{XH} * \mathrm{YT}$ |
| 50 |  | CALL ADDACC (P,XYSUM) |
| 51 |  | $\mathrm{P}=\mathrm{XH} * \mathrm{YH}$ |
| 52 |  | CALL ADDACC (P,XYSUM) |
| 53 |  | RETURN |
| 54 |  | END |

The additions are accomplished by the ADDACC subroutine, which is listed on the next page. ADDACC begins $24-30$ by putting the larger of $P$ and XYSUM(1) in $U$ and the smaller in V . This is to minimize cancellation error in the calculation 36 of $\mathrm{U}-\mathrm{Z}$ (if U is close to $\mathrm{Z}=\mathrm{U}+\mathrm{V}$ then little or no shifting will be needed to align the binary points in finding $U-Z$ ). Then 33 we find $\mathrm{Z}=\mathrm{U}+\mathrm{V}$. Here some of the less-significant fraction bits of V are probably lost because V must be shifted to align its binary point with that of $U$. How much error does that introduce? The difference $\mathrm{U}-\mathrm{Z}$ should be exactly -V , but because of cancellation it will differ from -V by the error we seek. This is calculated 36 as ZZ . To that we add 39 the current contents of the least-significant doubleword of the accumulator. If the least-significant doubleword has grown big enough to be noticed if we added it to the most-significant doubleword, we want to move that much of it there. So the most-significant doubleword of the accumulator then becomes 42 the imprecise sum plus the correction to the sum plus the least significant doubleword of the accumulator. Finally 45 we replace the least-significant doubleword of the accumulator with the (small) amount that is necessary to make XYSUM(1)+XYSUM(2) equal to the corrected sum $\mathbf{Z}+\mathrm{ZZ}$. The complicated process just described has the effect of adding P to XYSUM at $2 \times 52=104$ bits of precision, which is almost the 112 bits of precision we would get if we were able to use REAL*16 arithmetic.

```
    SUBROUTINE ADDACC(P, XYSUM )
C This routine adds P to the extra-precision accumulator XYSUM.
    It must be compiled with optimization turned off.
    variable meaning
    DABS Fortran function returns |REAL*8|
    P quantity to be added to the accumulator
    U the larger in absolute value of P and XYSUM
    V the smaller in absolute value of P and XYSUM
    XYSUM the accumulator
    Z most significant part of sum
    ZZ least significant part of sum
    formal parameters
    REAL*8 P,XYSUM(2)
    local variables
    REAL*8 U,V,Z,ZZ
C
C -------------------------------------------------------------------------
C
C put the larger quantity in U and the smaller in V
    IF(DABS(XYSUM(1)) .LT. DABS(P)) THEN
        U=P
        V=XYSUM (1)
    ELSE
        U=XYSUM(1)
        V=P
    ENDIF
    find the sum, imprecisely
    Z=U+V
        compute the error that was made by rounding U+V to REAL*8
        ZZ=(U-Z)+V
        add to it the least significant part of the accumulator
        ZZ=ZZ+XYSUM(2)
        that might be enough to increase the most significant part
        XYSUM(1)=Z+ZZ
        make the least significant part of accumulator what is left
        XYSUM(2)=(Z-XYSUM(1))+ZZ
        RETURN
        END
```

The DDOTQ function listed on the next page uses MPYACC to compute a dot product using extra-precision accumulation. After doing some sanity-checking 23-24 it initializes the accumulator XYSUM to zeros $27-28$. Instead of the multiply-and-add loop we had before we now have 29-31 a loop of calls to MPYACC. On each invocation that routine computes $\mathrm{X}(\mathrm{J}) \times \mathrm{Y}(\mathrm{J})$ and adds it to the accumulator as described above. When the loop is finished we find the dot product 34 by adding together the most- and least-significant doublewords of the accumulator.

The program below compares DDOTQ to DDOT for finding a troublesome dot product.

```
    REAL*8 X(101),Y(101),DDOT,ANS,DDOTQ,ANSQ
    X(1)=1.D+08
    Y(1)=1.D+08
    DO 1 J=2,101
        X(J)=DFLOAT(J-1)
        Y(J)=1.D0/DFLOAT(J-1)
    1 CONTINUE
    ANS=DDOT (X,Y, 101)
    ANSQ=DDOTQ (X,Y,101)
    WRITE (6,901) ANS,ANSQ
901 FORMAT('DDOT finds ',1PD23.16/
    ; 'DDOTQ finds ',1PD23.16)
        STOP
    END
```

The program manufactures the following problem.

$$
\begin{aligned}
\mathbf{x} & =\left[10^{8}, 1,2,3, \ldots, 100\right] \\
\mathbf{y} & =\left[10^{8}, 1, \frac{1}{2}, \frac{1}{3}, \ldots, \frac{1}{100}\right] \\
\mathbf{x}^{\top} \mathbf{y} & =10^{16}+(1 \times 1)+\left(2 \times \frac{1}{2}\right)+\left(3 \times \frac{1}{3}\right)+\cdots+\left(100 \times \frac{1}{100}\right)=10000000000000100
\end{aligned}
$$

When the program is compiled with gfortran and run, it produces the following output. The product of the first two terms, $10^{16}$, is big enough so that the subsequent terms contribute nothing to the sum when DDOT does the calculation using REAL*8 arithmetic. However, when DDOTQ does the calculation using extra-precision accumulation the correct result is obtained.

```
unix[1] a.out
DDOT finds 1.0000000000000000D+16
DDOTQ finds 1.0000000000000100D+16
unix[2]
```

This chapter has introduced two-part values, which can be used to perform fixed-point arithmetic with numbers too big to store in an INTEGER*4, and extra-precision accumulation for computing floating-point dot products more precisely than we can by simply doing REAL*8 arithmetic. It is also possible to use Classical Fortran for integer calculations of arbitrary precision, as described for example in [12, §20.6], and for floatingpoint calculations of arbitrary precision by invoking Brent's multiple precision package (see https://maths-people.anu.edu.au/~brent/pub/pub043.html).

```
    FUNCTION DDOTQ(X,Y,N)
    This routine computes the dot product of X with Y,
    using extra-precision accumulation.
    variable meaning
    J index on the elements of X and Y
    MPYACC routine does extra-precision multiply and accumulate
    N number of elements in X and Y
    X one of the vectors in the dot product
    XYSUM extra-precision result
    Y the other vector in the dot product
    formal parameters
    REAL*8 DDOTQ,X(N),Y(N)
    local variable
    REAL*8 XYSUM(2)
C check for a sensible value of N
    DDOTQ=0.DO
    IF(N.LE.0) RETURN
    accumulate the product at extended precision
    XYSUM(1)=0.DO
    XYSUM(2)=0.DO
    DO 1 J=1,N
            CALL MPYACC(X(J),Y(J), XYSUM )
    1 CONTINUE
        return a double-precision answer
        DDOTQ=XYSUM(1)+XYSUM(2)
        RETURN
        END
```

C
C
C
[201] Stokes, H. H., "The sensitivity of econometric results to alternative implementations of least squares," Journal of Economic and Social Measurement 30 (2005) 9-38. In the source code of Stokes' B34S program, this approach to implementing the extra precision accumulation idea is attributed to "1980 IMSL code that is no longer supported."
[202] Muller, Jean-Michel; Brisebarre, Nicolas; de Dinechin, Florent; Jeannerod, Claude-Pierre; Lefèvre, Vincent; Melquiond, Guillaume; Revol, Nathalie; Stehlé, Damien; and Torres, Serge, Handbook of Floating-Point Arithmetic, Birkhäuser, 2010.

## 18.5+ Generating Pseudorandom Numbers

Some scientific and engineering calculations are best performed by means of simulation $[53, \S 13]$ in which random trials are used to approximate the solution of a deterministic problem or the random behavior of a real system is modeled by a computer program. Either sort of simulation requires a sequence of numbers that appear to be random. Among the many algorithms that have been proposed for generating such a pseudorandom sequence, the mixed congruential algorithm

$$
x_{k}=\left(a x_{k-1}+b\right) \bmod 2^{31}
$$

[9, $\S 3]$ is the most widely used. It is simple enough to provide a nice example of Fortran programming and it is interesting because of the trivial way in which its modulus operation can be performed, so it makes an appearance in Exercises 4.10.48, 6.8.20, and 8.8.20 of this book. You might wish to reread the first of those now.

Depending on the numbers chosen for $a$ and $b$ the mixed congruential algorithm can generate up to $2^{31}$ numbers before the sequence begins to repeat, but some simulations use more. The generalized shift register algorithm

$$
x_{k}=x_{k-147} \oplus x_{k-250}
$$

[53, §13.3] [203], in which $\oplus$ denotes the bitwise xor operation (see §4.6.3), generates $2^{250}-1$ values before it repeats. It requires that we remember the previous 250 numbers that have been generated, which makes it also interesting but not so simple as the mixed congruential algorithm. To see how this algorithm can be implemented, imagine that we have already filled the circular shift register $S$ pictured below with 250 randomly-generated seeds $s_{1} \ldots s_{250}$, five of which are shown. If we let $x_{k-147}=s_{148-k}$ and $x_{k-250}=s_{251-k}$ then we can compute $x_{1}=s_{147} \oplus s_{250}$ as shown.


Then we can remember $x_{1}$ by using it to replace $s_{250}$, and compute $x_{2}=s_{146} \oplus s_{249}$ as illustrated below.


The vectors pointing from $x_{k-250}$ and $x_{k-147}$ to the exclusive-or symbol at the center of the circle rotate clockwise together as successive $x_{k}$ are produced, through $k=147$ when $148-k=1,251-k=104$, and $x_{147}=s_{1} \oplus s_{104}$. To find $x_{148}$ the vectors rotate one more element clockwise as shown below, so $x_{148}=s_{0} \oplus s_{105}=s_{250} \oplus s_{105}$.


Here is a pseudocode description of the process pictured above, in which I have assumed that n numbers are to be generated.

```
initialize pointers
km250=251
km147=148
do k=1,n
    rotate the vectors one element clockwise
    km250=km250-1
    if(km250=0) km250=250
    km147=km147-1
    if(km147=0) km147=250
    compute the result
    x (k) =s (km250) }\oplus\textrm{s}(\textrm{km}147
    and save it in the shift register for use later
    s(km250)=x(k)
enddo
```

The variable km250 represents $k-250$ and km 147 represents $k-147$. The first pass of the loop decrements these pointers to have the values 250 and 147 respectively and computes $x_{1}=s_{250} \oplus s_{147}$, the second pass of the loop makes km250=249 and km147=146 and computes $x_{2}=s_{249} \oplus s_{146}$, and so on. Each time a seed $\mathrm{s}(\mathrm{km} 250)$ is used to compute a new $x_{k}$ it is replaced by that new value. Eventually decrementing km147 gives it a value of zero, but as shown in the third diagram above the element of $S$ that should enter the calculation is not $s_{0}$ but $s_{250}$ (in which we stored the previous value we calculated for $x_{1}$ ) so km147 is reset to 250 . When the vector pointing from $x_{k-250}$ rotates past $s_{1}$ to $s_{0}$ the variable km250 is similarly reset from 0 to 250 . You should convince yourself that the loop in this pseudocode faithfully describes the rotation of the vectors in the pictures shown above and thus the calculation of the successive $x_{k}$.

To be useful in a simulation the pseudorandom values we generate must be floating-point numbers uniformly distributed on the closed interval from 0 to 1 . Sequences generated using the generalized shift register algorithm have been shown [203, pp519-523] to be statistically indistinguishable from those drawn from a uniform distribution, but making our Fortran implementation of the algorithm produce REAL*8 numbers in the right range entails several complications.

First, the built-in Fortran function IEOR discussed in $\S 4.6 .3$ operates on bitstrings that are stored in INTEGER*4 variables. To generate one REAL*8 number we must XOR two pairs of INTEGER*4 numbers and store the two-word result in the same memory occupied by the REAL*8 we want.

Second, the magnitude of the REAL*8 is determined by its most significant 12 bits, which represent its sign and exponent. Recall from $\S 4.2$ that the value of such a number is

$$
r=(-1)^{s} \times 2^{p-1023} \times(1+f)
$$

where $s$ is the sign bit, $p$ is the exponent represented by the next 11 bits, and $f$ is the binary fraction. The bits of $f$ should be randomly generated, but for $r$ not to exceed 1 we must set $s=0$ and $p=1023$ in each number we generate and subtract 1 from the result.

Third, because we will be manipulating the bits of the floating-point number representation, we must pay attention to the order in which the bytes are stored. Recall from $\S 4.8$ that on a little-endian processor it is the most-significant byte of a number that is stored at the lowest address.

The subroutine DR250 listed on the next two pages takes account of all these considerations. The internal shift register ISR is initialized at compile time with seeds 49-298 that are suitable for many applications.

If the routine is invoked with $N>0$ the contents of the shift register are used 305-325 to generate N random numbers in X . The DO 2 loop is a practical version of the idealized pseudocode given above. Each iteration of the loop generates 321-322 two INTEGER*4 bitstrings IX (1) and IX (2), which 45 occupy the same memory as the REAL*8 quantity XK and are thus the two halves of that doubleword; subtracting 1.D0 from it 323 yields the normalized result $X(K)$. This code is intended for a little-endian processor (such as those in the Intel Pentium family 320 ) so IX (1) and IX (2) are respectively JX (2) and JX (1) ; to revise it for a big-endian processor it is necessary only to make these assignment statements not reverse the order of the words. The fullwords JX (1) and JX (2) are made 318-319 from the adjacent shift register elements ISR ( $2 * \mathrm{KM} 250-1$ ) and ISR ( $2 *$ KM250) , which together make up the doubleword that we called s(km250) in the pseudocode. JX (2) is just the second half of the doubleword 319 but the first half of the doubleword needs to begin with the bit pattern for a REAL*8 number that is in the interval $[0,1]$; this is achieved 318 by OR-ing the fullword with the bit pattern in MASKC 42 . The updating of s (km250) indicated in the pseudocode is accomplished here by (very fast) IEOR operations 314-315 on the ISR elements. When DR250 is used in this way it returns with $N$ unchanged.

If the routine is invoked with $N \leq 0$ the shift register is reloaded $339-354$ with values obtained using the particular mixed congruential algorithm described in $[5, \S 10.1]$, and X is left unchanged. Each iteration of the DO 4 loop performs the calculations of the mixed congruential algorithm for the first $342-344$ and then the second $347-349$ fullword of that element in the shift register. Each result is AND-ed with MASKZ to zero its high-order bit, making it a positive integer; the high-order word is first AND-ed with MASKX to set its characteristic to zero so that the REAL*8 value of which it is a part will be in the range $[0,1]$. After DR250 is invoked in this way to reload the internal shift register, it can then be called a second time with $N>0$ to generate a random vector $X$ (see its man page).

If $N<0$ on input the starting value used for the reloading process is $329|N|$ and on return $N$ contains 351 the negative of the final value resulting from the reloading process.

If $N=0$ on input, the starting value for the reloading process is obtained 331-336 from the time-of-day clock and on return N contains the negative of that value. First 331 GETIMEOFDAY (see $\S 18.5 .3$ ) obtains the two-part value TOD containing the seconds and microseconds elapsed since midnight. Each of these is used as the starting value for one iteration $332-333$ of the mixed congruential algorithm. Then $N$ is found 334 as their exclusive-or. This sequence of operations reliably produces a large integer having an irregular bit pattern; to ensure that it is negative and nonzero, the result is or-ed 335 with NODD 36 .

The long repetition period and high execution speed of DR250 make it suitable for many large simulations.
[203] Kirkpatrick, Scott. and Stoll, Erich P., "A Very Fast Shift-Register Sequence Random Number Generator," Journal of Computational Physics 40 (1981) 517-526.

Copyright © 2024 Michael Kupferschmid, all rights reserved.
This supplementary textbook Section is licensed under CC-BY 4.0. Anyone who complies with the terms specified in
https://creativecommons.org/licenses/by/4.0/legalcode.txt
may use the work in the ways therein permitted.

| 1 |  | SUBROUTINE DR250 ( $\mathrm{N}, \mathrm{X}$ ) |
| :---: | :---: | :---: |
| 2 |  | This routine generates a vector X of N normalized |
| 3 |  | double-precision pseudorandom numbers in the interval [0,1] |
| 4 |  |  |
| 5 |  | variable meaning |
| 6 |  | -------- ------- |
| 7 | C | A multiplier for mixed congruential algorithm |
| 8 | C | C increment for mixed congruential algorithm |
| 9 | C | GETIMEOFDAY unix routine returns time of day and time zone |
| 10 | C | IABS Fortran function gives \|INTEGER*4| |
| 11 | C | IAND Fortran function gives bitwise AND of fullwords |
| 12 | C | IEOR Fortran function gives bitwise XOR of fullwords |
| 13 | C | IOR Fortran function gives bitwise OR of fullwords |
| 14 | C | ISR internal shift register |
| 15 | C | IX a doubleword of X as 2 singlewords |
| 16 | C | JX IX with the words switched |
| 17 | C | $\mathrm{K} \quad$ index on random numbers generated |
| 18 | C | KM147 index in ISR of doubleword K-147 |
| 19 | C | KM250 index in ISR of doubleword K-250 |
| 20 | C | MASKC to set characteristic of ISR values generated |
| 21 | C | MASKX to zero characteristic of ISR values generated |
| 22 | C | MASKZ to zero the high-order bit of a word |
| 23 | C | N number of random values needed, or seed (see above) |
| 24 | C | NODD to make SEED end-bits ones |
| 25 | C | TOD time-of-day [seconds,microseconds] |
| 26 | C | SEED seed used for mixed congruential algorithm |
| 27 | C | SET T => N has been set to -SEED for return |
| 28 | C | X vector of random values returned |
| 29 | C | XK a doubleword of X |
| 30 | C | ZONE unused; for GETIMEOFDAY |
| 31 | C |  |
| 32 | C | formal parameter |
| 33 |  | REAL*8 X (N) |
| 34 | C |  |
| 35 | C | prepare to seed the generator |
| 36 |  | INTEGER*4 SEED,TOD(2),ZONE (2),NODD/Z'80000001'/ |
| 37 |  | INTEGER*4 A/843314861/, C/453816693/ |
| 38 |  | INTEGER*4 MASKZ/Z'7FFFFFFF'/,MASKX/Z'000FFFFF'/ |
| 39 |  | LOGICAL*4 SET |
| 40 | C |  |
| 41 | C | prepare to run the generator |
| 42 |  | INTEGER*4 KM250/251/,KM147/148/,MASKC/Z'3FF00000'/ |
| 43 |  | REAL*8 XK |
| 44 |  | INTEGER*4 IX (2), JX (2) |
| 45 |  | EQUIVALENCE (XK, IX (1)) |
| 46 | C |  |
| 47 | C | internal shift register with values from SEED=123457 |
| 48 |  | INTEGER*4 ISR(500)/ |
| 49 |  | Z'0007E8AF', Z'D4C00D62', 248 lines of data |
| 298 |  | ; Z'0003731D', Z'8AD80548'/ |
| 299 | C |  |
| 300 | C |  |
| 301 C |  |  |

```
302 C
303
304 C
305 C
306
307 C
308
309
310
311
312 C
313 C
314
315
316 C
317 C
318
319
320 C
321
322
323
324
325
326 C
327 C
328
329
330
331
332
333
334
335
336
337
338 C
339 C
340
341 C
342
343
344
345 C
346 C
347
348
349
350
351
352
353
354
355
```

```
    is this an initialization call?
```

    is this an initialization call?
    IF(N.LE.0) GO TO 1
    IF(N.LE.0) GO TO 1
    generate N new random numbers while reseeding the generator
    generate N new random numbers while reseeding the generator
    DO 2 K=1,N
    DO 2 K=1,N
        find the indices in ISR of X(K-250) and X(K-147)
        find the indices in ISR of X(K-250) and X(K-147)
        KM250=KM250-1
        KM250=KM250-1
        IF(KM250.LE.0) KM250=250
        IF(KM250.LE.0) KM250=250
        KM147=KM147-1
        KM147=KM147-1
        IF(KM147.LE.0) KM147=250
        IF(KM147.LE.0) KM147=250
        exclusive-or the singlewords
        exclusive-or the singlewords
        ISR(2*KM250 )=IEOR(ISR(2*KM250 ),ISR(2*KM147 ))
        ISR(2*KM250 )=IEOR(ISR(2*KM250 ),ISR(2*KM147 ))
        ISR (2*KM250-1)=IEOR (ISR (2*KM250-1) , ISR (2*KM147-1))
        ISR (2*KM250-1)=IEOR (ISR (2*KM250-1) , ISR (2*KM147-1))
        extract the resulting doubleword
        extract the resulting doubleword
        JX(1)=IOR(ISR(2*KM250-1),MASKC)
        JX(1)=IOR(ISR(2*KM250-1),MASKC)
        JX (2) =ISR (2*KM250)
        JX (2) =ISR (2*KM250)
        the word order is reversed in the Pentium
        the word order is reversed in the Pentium
        IX (1)=JX (2)
        IX (1)=JX (2)
        IX(2)=JX(1)
        IX(2)=JX(1)
        X(K)=XK-1.D0
        X(K)=XK-1.D0
    2 CONTINUE
    2 CONTINUE
    RETURN
    RETURN
    get a seed to use in the reloading process
    get a seed to use in the reloading process
    1 SET=.FALSE.
1 SET=.FALSE.
SEED=IABS (N)
SEED=IABS (N)
IF(SEED.GT.0) GO TO 3
IF(SEED.GT.0) GO TO 3
CALL GETIMEOFDAY(TOD,ZONE)
CALL GETIMEOFDAY(TOD,ZONE)
TOD (1) =A*TOD (1)+C
TOD (1) =A*TOD (1)+C
TOD (2)=A*TOD (2)+C
TOD (2)=A*TOD (2)+C
N=IEOR(TOD (1) ,TOD (2))
N=IEOR(TOD (1) ,TOD (2))
N=IOR(N,NODD)
N=IOR(N,NODD)
SEED=-N
SEED=-N
SET=.TRUE.
SET=.TRUE.
reload the ISR using a mixed congruential algorithm
reload the ISR using a mixed congruential algorithm
3 DO 4 K=1,250
3 DO 4 K=1,250
low-order word of the 8-byte value
low-order word of the 8-byte value
SEED=A*SEED+C
SEED=A*SEED+C
ISR(2*K)=SEED
ISR(2*K)=SEED
SEED=IAND (SEED,MASKZ)
SEED=IAND (SEED,MASKZ)
high-order word of the 8-byte value
high-order word of the 8-byte value
SEED=A*SEED+C
SEED=A*SEED+C
ISR (2*K-1) =IAND (SEED,MASKX)
ISR (2*K-1) =IAND (SEED,MASKX)
SEED=IAND (SEED,MASKZ)
SEED=IAND (SEED,MASKZ)
4 CONTINUE
4 CONTINUE
IF(.NOT.SET) N=-SEED
IF(.NOT.SET) N=-SEED
KM250=251
KM250=251
KM147=148
KM147=148
RETURN
RETURN
END

```
    END
```


[^0]:    Copyright (c) 2024 Michael Kupferschmid, all rights reserved.
    This supplementary textbook Section is licensed under CC-BY 4.0.
    Anyone who complies with the terms specified in
    https://creativecommons.org/licenses/by/4.0/legalcode.txt
    may use the work in the ways therein permitted.

