Computer System Support for Scientific and Engineering Computation

Lecture 16 - June 23, 1988 (notes revised July 11, 1988)

1 Symbolic Math Systems

On the occasion of the announcement of Stephen Wolfram's *Mathematica* system, we give a brief overview of the field. Symbolic mathematics systems allow you to manipulate mathematical expressions symbolically rather than numerically. Thus evaluating $\int_0^\infty e^{-x^2}dx$ numerically would give you an approximation such as .886, whereas a symbolic system would compute the integral as "$\frac{\sqrt{\pi}}{2}$". Here are some of the common symbolic systems.

MACYSMA The first big symbolic system done at MIT, and written in lisp. A very large program, that has been worked on by many different people, and shows it.

REDUCE Originally written by Tony Hearn, and written in FORTRAN, so once considered more portable than MACSYMA. Also a very large system that has been continually extended.

Maple Done at Waterloo, and writen in C, although it has a lisp-like interface. Has a better overall design than MACSYMA or REDUCE.

MuMath Runs on IBM PC, and has mostly slow algorithms. However, it comes with a lisp-like language that can be used to reprogram its algorithms, and it is decomposable into small modules.

Mathcad This is not a true symbolic math system. It accepts symbolic expressions, but is really just a front end to a numerical analysis system.

One convenient feature of MACSYMA and Reduce is that they can directly generate FORTRAN code.

2 Floating Point Precisions

It is extremely rare for real-life problems to require more than double precison. The few cases that appear to require quadruple precision can usually be done in double precision using a better algorithm. For example, we saw that compensated summation is a way to obtain almost the effect of quadruple precision when summing a large number of double precision quantities. Another example is least squares. The naive algorithm might appear to require quadruple precision, but there is a trick (to be explained later) that enables the calculation to be done in double precision. An explanation for why double precision is almost always enough, is that final answers are rarely needed to more than 1 part in a million, which can be expressed in single precision. The rule of thumb we have noted earlier says that to get a final answer accurate to single precision, it is enough to carry the intermediate results in double precision.

2.1 Effect of Precision on Software

Besides the obvious fact that higher precision will almost always result in higher accuracy, precision enters into numerical calculations in more subtle ways. In algorithms that use iteration, the two factors that enter into stopping criteria are *noise* (rounding errors) and precision. Thus it is important for such a program to know exactly what precision is being used, and very helpful if double and single precision are genuinely different. For example, a program that uses double precision in an iteration to produce a single precision result might halt when a difference of two double precision numbers is 0 when computed to single precision accuracy. If single and double precision are identical (either in hardware or because a compiler converted all floating point operations to double), such programs won't work properly.

Another example where precision enters calculations is in finding the roots of a quadratic. We saw that it is important that the difference $B^2 - AC$ be computed in twice the precision of the desired result. Programmers will typically assume that double precision has at least twice the precision of single precision, and that computing $B^2 - AC$ in double yields a final result for the zeros accurate to single precision. But machines have been built where double precision has less than twice the precision of single precision (this is explicitly forbidden in the IEEE standard).

2.2 What IEEE says about precision

One of the goals of the IEEE floating point standard was to make debugging easier by having different machines produce exactly the same bits. Imagine two machines. The first is one like the Motorola 68881 or Intel 8087, that always produces results to double extended precision. The second is a machine like the ELXSI 6400, that produces results to the same precision as the operands. A double precision operation on the ELXSI can be simulated exactly on the 68881 if the 68881 rounds to double. The IEEE standard requires that such a rounding mode be provided. It is not sufficient to first compute the result in extended (that is compute as if to an infinite number of places and then round to extended) and then round that to double precision, because this double rounding may not produce exactly the same bits as rounding immediately to double precision in the first place.[1] Of course, it might be necessary to use assembly language to change the rounding mode.

So, the IEEE standard requires that when performing an operation on arguments of a given precision, it must be possible to produce the result in that same precision, possibly by changing a rounding mode. Conversely, the IEEE standard prohibits rounding the result to a precision smaller than the precision of the operands. The reason is again to facilitate comparisons between machines. If "narrow" rounding were allowed, then when two extended

[1] As we saw in an earlier lecture, double rounding will not change the answer when rounding first to double and then to single precision.

operands were combined to form a double precision result, there would be confusion as to whether the operation was first computed to extended and then rounded, or whether the operation was rounded just once to double. By prohibiting "narrow" rounding, you know that the result must have been double rounded. Thus when comparing the results of two machines that conform to the IEEE standard, you know that they must both double round and the two results should be bit for bit compatible.

There are two objections to this argument. The first is that IEEE 854 does not specify the number of bits for single, double and extended. And even IEEE 754 only specifies the bits for single and double, but not for extended precision. So if two different machines use different sizes for single precision, then you can't do bit for bit comparison, so what would be the point of controlling rounding? Of course, many machines (in fact most implementing the IEEE standard) use IEEE 754 for single and double, and use 80 bits for double extended. The second objection has to do with transcendental functions. The IEEE standard doesn't say anything about them. Since most real calculations involve computing transcendentals, bit for bit comparison is meaningless for them.

Why doesn't the IEEE standard define transcendental operations the way it defines addition, multiplication and square roots? The reason is the *table-maker's dilemma*. Suppose you are making a table of natural logs to 4 places. Then $\ln(.942) = -0.05975$. Should this be rounded to .0597 or .0598? If we compute ln(.942) more carefully, we get -0.059750. And then -0.0597500. And then -0.05975000. Since ln is transcendental, this could go on arbitrarily long. Thus it is not practical to specify transcendental functions to be computed as if to infinite precision and then rounded. We could try to specify transcendental functions algorithmically. But there does not appear to be a single algorithm that works well across all hardware architectures. For some hardware CORDIC is the best choice. For others, rational approximations are best. For still others, large tables are most appropriate. At present no single algorithm works acceptably over the wide range of current hardware; that may change.

2.3 Precision of Intermediate Results

One of the gray areas in most language specifications concerns the precision to be used in evaluating anonymous intermediate expressions. Consider the FORTRAN expression `D = D + U[i]*V[i]`, where `D` is double precision, and the other variables are single. Early FORTRAN compilers would multiply the two single precision variables `U[i]` and `V[i]` to get a double precision result, and add that to `D` with a double precision add. This was very useful for computing inner products, since when the array is long, the long summation can cause quite a bit of roundoff error if computed in single precision. Modern FORTRAN compilers are much more likely to do the minimum amount of work required by the FORTRAN standard, and compute `U[i]*V[i]` to single precision, since that is the type of both arguments. They do provide however, a `DPROD` function so that `D + DPROD(U[i],V[i])` has the desired effect.[2] This brings up the question of how to evaluate expressions. There are three basic strategies:

Strict Evaluation This is the method that gives a strict interpretation to the FORTRAN standard. Each expression is computed to the maximum precision of its two operands. This works well on "orthogonal" machines like the VAX, IBM 370,[3] ELXSI 6400 and

[2]Besides the DPROD cluttering up the code, it also *requires* double precision, which is quite expensive on Cray class machines.

[3]Except for the special case of DPROD, which the 370 can do in hardware.

NS 32081, which for every combination of an arithmetic operation and a precision, has a corresponding instruction. It does not evaluate an expressions like `S = D + U*V` in the way most likely intended by the programmer.

Widest Available This is the method required by the original C language. Each expression is computed in the machine's widest precision. This works well on the Motorola 68881, Intel 8087, and WE 32106, which always compute results to extended precision. However, on machines for which computing in the highest precision is significantly more expensive than single precision, it is not only inefficient but often does not result in significantly better accuracy.

Scan for Widest This scans an expression for the widest operand, and computes the entire expression in that precision. There is a subtlety with expressions involving a non-generic operator such as `SINGLE`. In the expression `S + SINGLE(D - E)` where `D` and `E` are double and `S` is single precision, the addition should be done in single precision, even though the expression does contain a double.

Compilers should implement either "Widest Available" or "Scan for Widest". It is important that compilers document which approach they use, and useful if they offer a compiler option that selects between the two approaches.[4]

2.4 Hardware Precision Paradigms

There are two major categories of computers widely used for floating point. The DEC VAX, IBM 360/370 and HP Precision architecture families offer single and double precision, with a single precision of about 24 bits, and double precision of about 53 significant bits.[5] The Cray and CDC machines on the other hand, had initially only one precision in hardware (single), which is roughly equivalent to double precision in the first category. For the most part, they must do double precision in software, which is dramatically slower than single precison. That is, the ratio of double precision execution time to single precision execution time is small in the first category, and large in the second. Since FORTRAN requires that the size of a float be the same size as an integer, it is hard for FORTRAN programs to make use of a 32 bit floating point format on the second category of machines, even when there is some hardware support for half precision.

Highly portable software must run well on both classes of machines. The usual solution is to write portable routines in two versions, a single precision version and a double precision one. On Cray class machines, the single precision routine is the one that will almost always be wanted, since single precision is already 48 significant bits, and double precision is dramatically slower. On the first category of machines, it will be quite common to run the double precision version. This classification of machines also effects the decision on how to evaulate `D = D + U[i]*V[i]`. When double precision is expensive, accumulating in double precision is probably a bad choice, whereas on the first class of machines, accumulating in double precision is usually prefered. This is an argument in favor of letting the compiler decide in which precision to evaluate `D = D + U[i]*V[i]` rather than forcing it with `DPROD`.

A final observation about precision. Some numerical problems are more demanding of floating-point hardware than others. The least demanding tend to be matrix problems and

[4] A reference for this material is Farnum's paper *Compiler Support for Floating-Point Computation*.

[5] On IBM machines, the exponent range is the same for all precisions, so the smallest number that can be represented is about 2^{-256}. This means that in quad precision, ϵ^4 will underflow, where ϵ is the roundoff error. The same is true of the DEC VAX D-format double-precision, but G-format is O.K.

partial differential equations solved by difference or finite element methods. These work well even on machines with poor floating point accuracy like the Cray, where the roundoff error for multiplication is 8 times the roundoff error for addition and subtraction. Thus users who primarily solve such problems will usually be more interested in floating point speed than in fine points about precision.

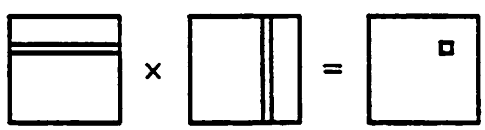
3 Matrix Double Precision Accumulation

We have discussed how accumulating sums in double precision improves the accuracy of inner products, and how compilers can help with this situation by generating double precision multiplies for `D = D + U[i]*V[i]`. When the inner product computation is done as part of a matrix multiplication, the issue of page (and cache) misses can be important. The straightforward method of multiplying two matrices is

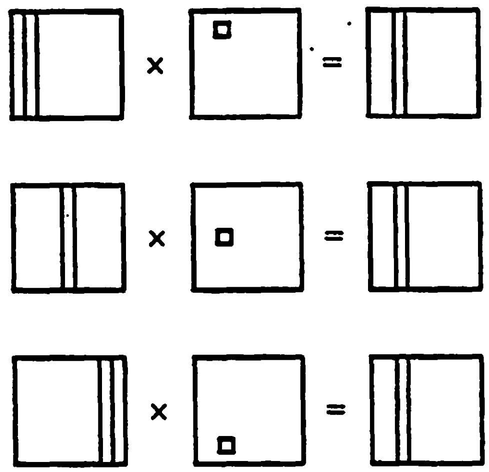
```
/* Algorithm 1 */
double T;

for i = 1 to N {
    for j = 1 to N {
        T = 0.0;
        for k = 1 to N
            T = T + A[i,k]*B[k,j];
        C[i,j] = T;
    }
}
```

Accumulating the sums of products in double precision does not result in any extra memory traffic, because the array arguments `A[i,k]` and `B[k,j]` are fetched as single precision quantities, and the result of the multiplication and double precison add is stored into T, which presumably is allocated to a register. In a picture, matrix multiplication looks like this:



To get the (i,j)th element of the product, you take the inner product of the ith row with the jth column. In FORTRAN, arrays are stored in column order. That means that the elements of the jth column will all be located in the same area of memory, but the ith row will be scattered. If the array is large, this will result in cache misses or even page misses because of the non-local memory references. Another way to organize the calculation of two matrices is to rewrite the equation $c_{ij} = \sum_k a_{ik}b_{kj}$ as $\vec{c}_j = \sum_k \vec{a}_k b_{kj}$ where the matrix A is decomposed into columns $A = (\vec{a}_1, \ldots, \vec{a}_n)$, and similarly for C. The sum isn't computed all at once, but rather gradually as indicated in the following picture.



Each row of the picture represents a vector $\vec{a}_k b_{kj}$ being added to the indicated column of C. Thus the multiplication algorithm looks something like this

```
/* Algorithm 2 */
for j = 1 to N {
    for i = 1 to N
        T[i] = 0.0;
    for k = 1 to N {
        BKJ = B[k,j];
        for i = 1 to N
            T[i] = T[i] + A[i,k]*BKJ;
    }
    for m = 1 to N
        C[m,j] = T[m];
}
```

To compare the page faults generated by the two methods, imagine a page size of 4096 bytes and a 1024 by 1024 matrix of 4 byte single precision numbers. Thus each page will hold 1 column, and each matrix fits into 1024 pages. Also imagine that the working set is less than 1024 pages (that is, less than 4 megabytes). In the inner loop of algorithm 1, all the `B[k,j]` will fit into one page, but the `A[i,k]` will touch each column of A, causing about 1024 page faults. To compute the entire product will cause about $1024(1024)^2$ page faults. In algorithm 2, the inner loop references a single column of A, touching one page. The loop on `k` sweeps through A touching 1024 pages, and the loop on `m` touches a single column of C. Thus each trip through the `j` loop touches about 1024 pages, for a total of 1024^2 page faults. Roughly speaking, algorithm 1 generates N^3 page faults, and algorithm 2 generates N^2 faults.

Although algorithm 2 dramatically reduces page faults, it changes the cost of doing double precision accumulation. In algorithm 1, double precision sums were accumulated in the variable T which could be assigned to a register. In algorithm 2, the double precision sums are accumulated in an array `T[i]`. Reading and writing this double precision array requires twice the memory bandwidth of single precision accumulation. The reader might want to ponder whether there is an algorithm that combines the low page fault cost of algorithm 2 with the low double precision accumulation cost of algorithm 1.[6] For Gaussian elimination, there is such an algorithm, and it is explained in Appendix A (*Gaussian Elimination with Extra-Precise Accumulation of Products*).

[6]If the matrix B can be cheaply transposed from column order to row order, then algorithm 1 no longer has a high page fault cost.

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Appendix A

GAUSSIAN ELIMINATION with EXTRA-PRECISE ACCUMULATION of PRODUCTS

– is it worth the cost ? –

W. Kahan

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Issues:

1. How to do it?
   - (a) Extended precision sums in inner loops. (Fast and cheap)
   - (b) Extended precision temporary vectors. (Slowed by memory)
2. What good is it?
   - (a) More accuracy in "systematically ill-conditioned" cases, almost as good as if all data were stored with a few extra bits; but otherwise the improvement is small.
   - (b) Error and its bound grows less quickly with dimension, so improvement is most apparent when dimension is huge.
3. What does it cost?
   - (a) Hardware is more complicated, but not much slowed.
   - (b) Subexpression semantics harder to compile.
   - (c) Method 1a may stumble over paging problems; this can be largely circumvented by trickery and some use of 1b.
4. Examples and comparisons:
   - (a) On 8087-like architectures (INTEL 86/330, IBM PC FORTH)
   - (b) Using software floating-point (hp-85, APPLE III)
   - (c) High-performance machines (ELXSI 6400, ...)
5. Programs listed below:

LUPA:	Triangular Factorization with extra-precise accumulation of inner products (method 1a), and alternative column-oriented code using extra-precise vector to accumulate scalar × vector products (method 1b).
LUXPB:	Forward and back sustitution by two methods, like LUPA.
RBAX:	Residual by two methods, like LUPA.
VNORM:	Root-sum-squares norm with extended-range accumulation of squares (method 1a), and alternative code using no extended range but three times slower.
RESYS:	Solve system of linear equations and refine solution iteratively, using LUPA, LUXPB, RBAX and VNORM.
HUPA:	A faster version of LUPA, and
HUXPB:	a faster version of LUXPB, to be used together in situations where page faults seem to preclude extra-precise accumulation of products.

LUPA:

Given a square matrix A, we seek triangular factors to satisfy

$$LU = PA,$$

where

L = unit lower triangular matrix,
U = upper triangular matrix, and
P = permutation matrix represented by indices $Ip[...]$
thus: $(Px)[i] = x[Ip[i]]$,
inverse(P) = transpose(P),
(inverse(P)y)$[i] = y[j]$ where $Ip[j] = i$.

If $i > j$ then

$$A[Ip[i], j] = L[i, j] * U[j, j] + \mathrm{Sum}\{k < j\}(L[i, k] * U[k, j])$$

else

$$A[Ip[i], j] = 1 * U[i, j] + \mathrm{Sum}\{k < i\}(L[i, k] * U[k, j]).$$

```
Subroutine LUPA( A, LU, Id, IP, N ):
    Integer values  Id, N ;  Integer variable  IP[N+] ;
    Real variables  A[Id,N+], LU[Id,N+] ; ... they may coincide.

    Integer  i, j, k, imax ;
    Logical  UnSav ; ... to save & restore Underflow flag.
    Real  cmax, dmax, rndf, undr,  U[N+] ;
    Tempreal tsum, tpmax, tsmax, T[N+] ; ... more precise than Real
    Equivalence  (U,T) ; ... Save storage by packing  U  inside  T .
    Common /L1BWSP/  T ; ... Shares workspace with other programs.

...Glossary:
...    A[Id,N+] is a square matrix dimensioned  A[Id, at least N ]
...    LU[Id,N+]  will hold  LU[i,j] = L[i,j]  for i>j ,
...                                  = U[i,j] otherwise .
...         ( The program allows  LU  to overwrite  A .)
...    IP[N+] will hold permuted indices  1, 2, 3, ..., N  thus:
...          (Px)[i] = x[IP[i]] .
...    j  is a column index that will run  1, 2, 3, ..., N .
...    U[N+]  will hold temporarily  column j  of  U .
...    T[N+]  will hold temporarily  (column j  of  L)*U[j,j] .
...    cmax holds the max. magnitude in column j  of  A .
...    dmax holds the max. subdiagonal magnitude in column j of PA
...    rndf = 1.000...0001 - 1  ,  measures roundoff among Reals.
...    undr = tiniest positive number ,  at or beyond underflow.
...    i  is a row index that will run  1, 2, 3, ..., N .
...    tsum = A[IP[i],j] - Sum{k}( L[i,k]*U[k,j] ) .
...    tsmax = max. |tsum|  in column j ;  if  tsmax/(8j) > cmax ,
...          U  has grown so big that roundoff may be excessive, so
...          columns 1 and j of  A  should be swapped. (Very rare.)
...    tpmax = max. subdiagonal |tsum|  in column j  for pivoting.
```

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```
...    imax = row index where  tpmax  occurs.

   UnSav := UndrflowFlag( .false. ) ; ... to save & reset U-flag.
...    Gradual Underflow during factorization is ignorable.

   rndf := 1.0 ; rndf := nextafter(rndf, 2.0) - rndf ;
...    or else try  rndf := 4.0 ;  rndf := rndf/3.0 ;
...                 rndf := abs( (rndf - 5.0/4.0)*3.0 - 1.0/4.0 ) ;
   undr := 0.0 ;  undr := nextafter(undr, 1.0) ;
...    or else try  undr := underflow threshold for the  Reals .

...    Initialize  IP :
   For  i = 1 to N do  IP[i] := i  ;

...    Outer loop, traversed once per column (j) :
   For  j = 1 to N ;
       cmax := 0.0 ;  tsmax := 0.0 ;
       ... Compute column j of U :
       For  i = 1 to j-1 ;
           tsum := A[IP[i], j] ;  cmax := max{ cmax, abs(tsum) } ;
           For  k =1 to i-1  do  tsum := tsum - LU[i,k]*U[k] ;
           U[i] := tsum ;  tsmax := max{ tsmax, abs(tsum) } ;
           next i ;

       ... Compute potential pivots :
       dmax := 0.0 ;  tpmax := 0.0 ;  imax := j ;
       For  i = j to N ;
           tsum := A[IP[i], j] ;  dmax := max{ dmax, abs(tsum) } ;
           for  k = 1 to j-1  do  tsum := tsum - LU[i,k]*U[k] ;
           T[i] := tsum ;  tsum := abs(tsum) ;
           if  tsum > tpmax then { imax := i ;  tpmax := tsum } ;
           next i ;
       cmax := max{ cmax, dmax } ;  tsmax := max{ tsmax, tpmax } ;
       If  imax = j  then {
           if  tpmax = 0.0  then {
               T[j] := max{undr, rndf*dmax} ;
               go to DivByPiv }
           }
       else { ... exchange rows  j  and  imax .
           for  k = 1 to j-1 ;  dmax := LU[imax,k] ;
               LU[imax,k] := LU[j,k] ;  LU[j,k] := dmax ;
               next k ;
           k := IP[imax] ;  IP[imax] := IP[j] ;  IP[j] := k ;
       }
       If tsmax/(8*j) > cmax  then {
           Display {"Warning: Extraordinary growth of
               intermediate results in  LUPA  may lose
               too much accuracy.  To avoid this loss,
```

```
                recompute after exchanging columns  1
                and  ", j } ;
            tsum := 0.0/0.0 ;  ...  signals  Invalid Operation.
        }
    DivByPiv:  tsum := T[imax] ;  T[imax] := T[j] ;  U[j] := tsum ;
        for  k = 1 to j  do  LU[k,j] := U[k] ;         ...  pivot.
        for  k = j+1 to N  do  LU[k,j] := T[k]/tsum ; ... = L[k,j].
        next  j ;
    UnSav := UndrflowFlag(UnSav) ; ... Restore Underflow flag.
    return ;
    end LUPA .
```

.... Alternative Column-Oriented Code ....

```
Subroutine LUPA( A, LU, Id, IP, N ):
    Integer values  Id, N ;  Integer variable  IP[N+] ;
    Real variables  A[Id,N+], LU[Id,N+] ; ... they may coincide.

    Integer  i, j, k, imax ;
    Logical  UnSav ; ... to save & restore Underflow flag.
    Real  cmax, dmax, smax, rndf, undr, z ;
    Tempreal  t, tpmax,  T[N+] ; ... more precise than Real
    Common /L1BWSP/  T ; ... Shares workspace with other programs.

...Glossary:
...    A[Id,N+] is a square matrix dimensioned  A[Id, at least N ]
...    LU[Id,N+]  will hold  LU[i,j] = L[i,j]  for i>j ,
...                                  = U[i,j] otherwise .
...         ( The program allows  LU  to overwrite  A .)
...    IP[N+] will hold permuted indices  1, 2, 3, ..., N  thus:
...           (Px)[i] = x[IP[i]] .
...    j  is a column index that will run  1, 2, 3, ..., N .
...    T[N+]  will hold temporarily  column j  of  U , and then it
...           will hold temporarily  (column j  of  L)*U[j,j] .
...    cmax holds the max. magnitude in column j  of  A .
...    dmax holds the max. subdiagonal magnitude in column j of PA
...    rndf = 1.000...0001 - 1  ,  measures roundoff among Reals.
...    undr = tiniest positive number ,  at or beyond underflow.
...    i  is a row index that will run  1, 2, 3, ..., N .
...    smax = max. |T[i]|  in column j ;  if  smax/(8j) > cmax ,
...          U  has grown so big that roundoff may be excessive, so
...          columns 1 and j of  A  should be swapped. (Very rare.)
...    tpmax = max. subdiagonal |T[i]|  in column j  for pivoting.
...    imax = row index where  tpmax  occurs.

    UnSav := UndrflowFlag( .false. ) ; ... to save & reset U-flag.
...    Gradual Underflow during factorization is ignorable.
```

```
    rndf := 1.0 ; rndf := nextafter(rndf, 2.0) - rndf ;
...    or else try  rndf := 4.0 ;  rndf := rndf/3.0 ;
...                 rndf := abs( (rndf - 5.0/4.0)*3.0 - 1.0/4.0 ) ;
    undr := 0.0 ;  undr := nextafter(undr, 1.0) ;
...    or else try  undr := underflow threshold for the  Reals .

...    Initialize  IP :
    For  i = 1 to N do  IP[i] := i  ;

...    Outer loop, traversed once per column (j) :
    For  j = 1 to N ;
        tpmax := cmax := dmax := smax := 0.0 ;
        ... Initialize column  T .
        For  i = 1 to N ;
            T[i] := z := A[IP[i], j] ;  z := abs(z) ;
            cmax := max{ cmax, z } ;
            if  i >= j  then  dmax := max{ dmax, z } ;
            next i ;

        For  k = 1 to j-1 ;  ... subtract U[k,j]*(col.k of L).
            LU[k,j] := z := T[k] ; ... = U[k,j] .
            smax := max{ smax, abs(z) } ;
            for  i = k+1 to N  do  T[i] := T[i] - LU[i,k]*z ;
            next k ;
        ...  Locate pivot  t ; it maximizes  |T[i]| .
        imax := j ;
        For  i = j to N ;
            t := abs(T[i]) ;
            if  t > tpmax then { imax := i ;  tpmax := t } ;
            next i ;
        If  imax = j  then {
            if  tpmax = 0.0  then {
                T[j] := max{undr, rndf*dmax} ;
                go to DivByPiv }
        }
        else { ... exchange rows  j  and  imax .
            for  k = 1 to j-1 ;  dmax := LU[imax,k] ;
                LU[imax,k] := LU[j,k] ;  LU[j,k] := dmax ;
                next k ;
                k := IP[imax] ;  IP[imax] := IP[j] ;  IP[j] := k ;
            }
        If max{ smax, tpmax }/(8*j) > cmax  then {
            Display {"Warning: Extraordinary growth of intermediate results
                in  LUPA  may lose too much accuracy.  To avoid this loss,
                recompute after exchanging columns  1  and  ", j } ;
            t := 0.0/0.0 ;  ...  signals  Invalid Operation.
        }
     DivByPiv:  t := T[imax] ;  T[imax] := T[j] ;
```

```
        LU[j,j] := t ; ... = pivot U[j,j] .
        for  k = j+1 to N  do  LU[k,j] := T[k]/t ; ... = L[k,j] .
    next  j ;
    UnSav := UndrflowFlag(UnSav) ; ... Restore Underflow flag.
    return ;
    end LUPA .
```

The two LUPA codes should give identical results, including roundoff, but at different speeds depending upon the dimension N and details of the machine's memory management. On a machine that accumulates products in a fast-access register, the first code should be the faster while N is so small that all data fits in a few pages and cache-blocks; otherwise the second code should be the faster, the more so as N increases. (Cf. HUPA below.)

LUXPB:

This program solves $LUX = PB$ for X given matrices
L = an unit lower triangular $N \times N$ matrix and
U = an upper triangular $N \times N$ matrix stored in LU thus:
if $i > j$ then $LU[i,j] = L[i,j]$ else $LU[i,j] = U[i,j]$.
B = an $N \times M$ matrix, and
P = an $N \times N$ permutation matrix represented by indices $Ip[i]$
thus: $(Px)[i] = x[Ip[i]]$.
X = an $N \times M$ matrix that will be calculated by solving in turn
$LC = PB, C[i,j] + \mathrm{Sum}\{k < i\}(L[i,k] * C[k,j]) = B[Ip[i],j]$
$UX = C, \mathrm{Sum}\{k \geq i\}(U[i,k] * X[k,j]) = C[i,j]$.
The solution X may overwrite B but not LU.

```
Subroutine  LUXPB( LU, Id, IP, N, B, X, M ):
    Integer values  Id, N, M ;  Integer variable  IP[N+] ;
    Real variables  LU[Id, N+],  B[Id, M+],  X[Id, M+] ;

    Integer  i, j, k ;
    Real  C[N+] ;
    Tempreal  tsum ; ... more precise than Reals .
    Common /L1BWSP/  C ;
    Logical UnSav ; ... Gradual Underflow matters only in  X .
    Unsav := UndrflowFlag(.false.) ;

    For  j = 1 to M ; ... solve for column  j  :
        for  i = 1 to N ;
            tsum := B[IP[i],j] ;
            for  k = 1 to i-1  do  tsum := tsum - LU[i,k]*C[k] ;
            C[i] := tsum ;
            next i ;
        for i = N to 1 step -1 ;
            tsum := C[i] ;
            for  k = i+1 to N  do  tsum := tsum - LU[i,k]*C[k] ;
            UnSav := UndrflowFlag(UnSav) ; ... Expose Underflow.
            X[i,j] := C[i] := tsum/LU[i,i] ;
```

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```
            UnSav := UndrflowFlag(UnSav) ; ... Hide Underflow.
            next i ;
         next j ;
      UnSav := UndrflowFlag(UnSav) ; ... Reveal  X 's  Underflows.
      return ;
      end LUXPB .
```

.... Alternative Column-Oriented Code ....

```
Subroutine  LUXPB( LU, Id, IP, N, B, X, M ):
    Integer values  Id, N, M ;  Integer variable  IP[N+] ;
    Real variables  LU[Id, N+],  B[Id, M+],  X[Id, M+] ;

    Integer  i, j, k ;
    Real  z ;                                                  ... *1
    Tempreal  C[N+] ; ... more precise than Reals .            ... *2
    Common /L1BWSP/  C ; ... shared workspace.
    Logical UnSav ; ... Gradual Underflow matters only in  X .
    Unsav := UndrflowFlag(.false.) ;

    For  j = 1 to M ; ... solve for column  j  :
        for  i = 1 to N  do  C[i] := B[IP[i],j] ;
        for  k = 1 to N ;
            z := C[k] ;  C[k] := z ;                           ... *3
            for  i = k+1 to N  do  C[i] := C[i] - LU[i,k]*z ;
            next k ;
        for k = N to 1 step -1 ;
            UnSav := UndrflowFlag(UnSav) ; ... Expose Underflow.
            X[k,j] := z := C[k]/LU[k,k] ;                      ... *4
            UnSav := UndrflowFlag(UnSav) ; ... Hide Underflow.
            for  i = 1 to k-1  do  C[i] := C[i] - LU[i,k]*z ;
        next k ;                                               ... *5
    next j ;
    UnSav := UndrflowFlag(UnSav) ; ... Reveal  X 's  Underflows.
    return ;
    end LUXPB .
```

*Notes: The foregoing two codes should produce identical results including the effects of roundoff. However, the second code can be modified slightly to give marginally more accurate results at no significant extra cost provided multiplication of Real by Tempreal costs at most negligibly more than Real by Real. First merge declarations ... *1 and ... *2 to read

```
Tempreal z, C[N+]; ... more precise than Reals. ... 1* & 2*
```

Next simplify statement ... *3 to read

```
z := C[k];                                           ... 3*
```

Finally, but only if references to UndrflowFlag() cost rather more than a handfull of memory references, replace ... *4 by

```
C[k] := z := C[k]/LU[k,k];                           ... 4*
```

and move the adjacent statements to bracket a new statement inserted after ... *5 thus:

```
next k;                                              ... *5

UnSav := UndrflowFlag(UnSav) ; ... Expose Underflow.
for i = 1 to N do X[i,j] := C[i];
UnSav := UndrflowFlag(UnSav) ; ... Hide Underflow.
next j; ... etc.
```

(Cf. HUXPB below.)

RBAX:

This program calculates a residual $R = B - AX$ given matrices
B = an $N \times M$ matrix,
A = an $N \times N$ matrix, and
X = an $N \times M$ matrix.

R may overwrite B but not A nor X.

```
Subroutine  RBAX( A, Id, N, X, M, B, R ):
    Integer values  Id, N, M ;
    Real variables  A, X, B, R ;

    Integer  i, j, k ;
    Tempreal  tsum ; ... more precise than Reals .

    For  j = 1 to M ; ... compute column  j .
        for  i = 1 to N ; ... row i .
            tsum := B[i,j] ;
            for  k = 1 to N  do  tsum := tsum - A[i,k]*X[k,j] ;
            R[i,j] := tsum ;
            next i ;
        next j ;
    return ;
    end RBAX .
```

.... Alternative Column-Oriented Code ....

```
Subroutine  RBAX( A, Id, N, X, M, B, R ):
```

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```
    Integer values  Id, N, M ;
    Real variables  A, X, B, R ;

    Integer  i, j, k ;
    Real  z ;
    Tempreal  T[N+] ; ... more precise than Reals .
    Common  /L1BWSP/  T ;  ... shared workspace.

    For  j = 1 to M ; ... compute column  j .
        for  i = 1 to N  do  T[i] := B[i,j] ;
        for  k = 1 to N ;  z := -X[k,j] ;
            for  i = 1 to N  do  T[i] := T[i] + A[i,k]*z ;
            next k ;
        for  i = 1 to N  do  R[i,j] := T[i] ;
        next j ;
    return ;
    end  RBAX .
```

<u>VNORM:</u>
For any $N \times M$ matrix B,

$$\begin{aligned} \text{VNORM}(B, Id, N, M) &= \| B \| = \text{SQRT}(\text{trace}(B^T B)) \\ &= \text{SQRT}(\text{Sum}\{1 \le j \le M, 1 \le i \le n\}(B[i,j])^2 \end{aligned}$$

where B is dimensioned $B[Id, M+]$.

```
Real Function  VNORM( B, Id, N, M ):
    Integer values  Id, N, M ;
    Real variable  B[Id, M+] ;
    Tempreal  t ;
    t := 0.0 ;
    for j=1 to M do  for i=1 to N do  t := t + B[i,j]**2 ;
    return  VNORM := SQRT(t) ;
    end  VNORM .
```

.... Alternatively, ...
if Tempreal is unavailable then the following code avoids over/underflow at the cost of some speed and accuracy.

```
Real Function  VNORM( B, Id, N, M ):
    Integer values  Id, N, M ;
    Real variable  B[Id, M+] ;
    Real  s, d, z ;
    Logical UnSav ; ... to save & restore Underflow flag.

    UnSav := UndrflowFlag(.false.) ;
    d := s := 0.0 ;
```

```
for  j = 1 to M ;  for  i = 1 to N ;
    z := abs( B[i,j] ) ;
    if  z > d  then {  s := s*(d/z)**2 + 1.0 ;  d := s  }
        else if  z > 0.0  then  s := s + (z/d)**2 ;
    next i ;  next j ;
UnSav := UndrflowFlag(UnSav) ; ... Ignore Underflows.
return  VNORM := d*SQRT(s) ;
end  VNORM .
```

RESYS:

This program uses iterative refinement to solve $AX = B$ and returns $RESYS = \| B - AX \|$, where

A = an $N \times N$ matrix dimensioned $A[Id, N+]$,
B = an $N \times M$ matrix dimensioned $B[Id, M+]$, and
X = an $N \times M$ matrix dimensioned $X[Id, M+]$.

```
Real Function  RESYS( A, Id, N, B, M, X ):
    Integer values  Id, N, M ;
    Real  A[Id, N+],  B[Id, M+],  X[Id, M+] ;

    Integer  i, j, k, L,   IP[N+] ;
    Real  Rold, Rnew, WS[ Id*(N+M+1)+ ] ;
    Common /L2BWSP/  WS ; ... shared work-space.
    Equivalence (IP,WS) ; ... packs  IP  inside  WS .

    Call LUPA( A, WS[Id+1], Id, IP, N ) ; ... LU = PA .
    Call LUXPB( WS[Id+1], Id, IP, N, B, X, M ) ; ... LUX = PB .
    Rold := 0.0 ;  L := 1+Id*(N+1) ;  Go to Residual ;

    Loop:  Rold := Rnew ;
        Call LUXPB( WS[Id+1], Id, IP, N, WS[L], WS[L], M ) ;
        ...   LUZ = PR , and  Z  overwrites  R  in  WS .
        For  j = 1 to M ; ...    do  X := X + Z .
            k := (N+j)*Id ;
            for i = 1 to N do  X[i,j] := X[i,j] + WS[k+i] ;
            next j ;
    Residual:  Call RBAX( A, ID, N, X, M, B, WS[L] ) ;
        ...   R = B - AX  in  WS .
        Rnew := VNORM( WS[L], Id, N, M ) ; ... = || R || .
        if ( Rold = 0.0  .or.  Rold > Rnew ) then go to Loop ;
    return RESYS :=  Rnew ;
    end RESYS .
```

Note: To make this code run faster on a paged machine when N is huge, replace LUPA and LUXPB respectively with HUPA and HUPXB respectively.

HUPA

Given an $N \times N$ matrix A, this program does the same as $LUPA$ except faster when N is very large. It calculates factors

$$LU = PA,$$

where

L = unit lower triangular matrix,
U = upper triangular matrix, and
P = permutation matrix represented by indices $Ip[...]$
thus: $(Px)[i] = x[Ip[i]]$.

If $i > j$ then
$A[Ip[i], j] = L[i,j] * U[j,j] + \text{Sum}\{k < j\}(L[i,k] * U[k,j])$
else
$A[Ip[i], j] = 1 * U[i,j] + \text{Sum}\{k < i\}(L[i,k] * U[k,j])$.

But, to diminish the performance degradation caused by page faults and other artifacts of memory management, $HUPA$ packs L thus:

$$L[i,j] = HU[N+1-i+j, N+1-i] \text{ for } i > j.$$

```
Subroutine HUPA( A, HU, Id, IP, N ):
    Integer values  Id, N ;  Integer variable  IP[N+] ;
    Real variables  A[Id,N+], HU[Id,N+] ; ... they must NOT overlap.

    Integer  i, j, k, imax, L ;
    Logical  UnSav ; ... to save & restore Underflow flag.
    Real  cmax, dmax, rndf, undr,  U[N+] ;
    Tempreal tsum, tpmax, tsmax, T[N+] ; ... more precise than Real
    Equivalence  (U,T) ; ... Save storage by packing  U  inside  T .
    Common /L1BWSP/  T ; ... Shares workspace with other programs.

...Glossary:
...     A[Id,N+] is a square matrix dimensioned  A[Id, at least N ]
...     HU[Id,N+]  will hold  HU[i,j] = L[N+1-j, i-j]  for  i > j ,
...                                   = U[i,j] otherwise .
...      ( The program expects  HU and A  NOT to overlap.)
...     IP[N+] will hold permuted indices  1, 2, 3, ..., N  thus:
...             (Px)[i] = x[IP[i]] .
...     j  is a column index that will run  1, 2, 3, ..., N .
...     U[N+]  will hold temporarily  column j  of  U .
...     T[N+]  will hold temporarily  (column j  of  L)*U[j,j] .
...     cmax holds the max. magnitude in column j  of  A .
...     dmax holds the max. subdiagonal magnitude in column j of PA
```

```
...     rndf = 1.000...0001 - 1   ,  measures roundoff among Reals.
...     undr = tiniest positive number ,  at or beyond underflow.
...     i  is a row index that will run  1, 2, 3, ..., N .
...     tsum = A[IP[i],j] - Sum{k}( L[i,k]*U[k,j] ) .
...     tsmax = max. |tsum|  in column j ;  if  tsmax/(8j) > cmax ,
...           U  has grown so big that roundoff may be excessive, so
...           columns 1 and j of  A  should be swapped. (Very rare.)
...     tpmax = max. subdiagonal |tsum|  in column j  for pivoting.
...     imax = row index where  tpmax  occurs.

    UnSav := UndrflowFlag( .false. ) ; ... to save & reset U-flag.
...     Gradual Underflow during factorization is ignorable.

    rndf := 1.0 ; rndf := nextafter(rndf, 2.0) - rndf ;
...     or else try  rndf := 4.0 ;  rndf := rndf/3.0 ;
...                  rndf := abs( (rndf - 5.0/4.0)*3.0 - 1.0/4.0 ) ;
    undr := 0.0 ;  undr := nextafter(undr, 1.0) ;
...     or else try  undr := underflow threshold for the  Reals .

...     Initialize  IP :
    For  i = 1 to N do  IP[i] := i  ;

...     Outer loop, traversed once per column (j) :
    For  j = 1 to N ;
        cmax := 0.0 ;  tsmax := 0.0 ;
        ... Compute column j of U :
        For  i = 1 to j-1 ;
            tsum := A[IP[i], j] ;  cmax := max{ cmax, abs(tsum) } ;
            L := N+1-i ;
            For  k =1 to i-1  do  tsum := tsum - HU[L+k,L]*U[k] ;
            HU[i,j] := U[i] := tsum ;
            tsmax := max{ tsmax, abs(tsum) } ;
            next i ;

        ... Compute potential pivots :
        dmax := 0.0 ;  tpmax := 0.0 ;  imax := j ;
        For  i = j to N ;
            tsum := A[IP[i], j] ;  dmax := max{ dmax, abs(tsum) } ;
            L := N+1-i ;
            for  k = 1 to j-1  do  tsum := tsum - HU[L+k,L]*U[k] ;
            T[i] := tsum ;  tsum := abs(tsum) ;
            if  tsum > tpmax then { imax := i ;  tpmax := tsum } ;
            next i ;
        cmax := max{ cmax, dmax } ;  tsmax := max{ tsmax, tpmax } ;
        If  imax = j  then {
            if  tpmax = 0.0  then {
                T[j] := max{undr, rndf*dmax} ;
                go to DivByPiv }
```

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```
        }
        else { ... exchange rows  j  and  imax .
            L := N+1-imax ;  i := N+1-j ;
            for  k = 1 to j-1 ;  dmax := HU[L+k,L] ;
                HU[L+k,L] := HU[i+k,i] ;  HU[i+k,i] := dmax ;
                next k ;
            k := IP[imax] ;  IP[imax] := IP[j] ;  IP[j] := k ;
        }
        If tsmax/(8*j) > cmax  then {
            Display {"Warning: Extraordinary growth of intermediate results
                in  HUPA  may lose too much accuracy.  To avoid this loss,
                recompute after exchanging columns  1  and  ", j } ;
            tsum := 0.0/0.0 ;  ...  signals  Invalid Operation.
        }
    DivByPiv:  tsum := T[imax] ;  T[imax] := T[j] ;
        HU[j,j] := U[j] := tsum ; ... = pivot U[j,j] .
        for  k = 1 to N-j  do  HU[j+k,k] := T[N+1-k]/tsum ;
        next  j ;                        ... = L[N+1-k,j] .
    UnSav := UndrflowFlag(UnSav) ; ... Restore Underflow flag.
    return ;
    end HUPA .
```

<u>HUXPB:</u>

This program solves $LUX = PB$ for X given matrices

L = an unit lower triangular $N \times N$ matrix and
U = an upper triangular $N \times N$ matrix stored in HU thus:
  if $i > j$ then $HU[i,j] = L[N+1-j, i-j]$
    else $HU[i,j] = U[i,j]$.
B = an $N \times M$ matrix, and
P = an $N \times N$ permutation matrix represented by indices $Ip[i]$
  thus: $(Px)[i] = x[Ip[i]]$.
X = an $N \times M$ matrix that will be calculated by solving in turn
  $LC = PB$, $C[i,j] + \text{Sum}\{k < i\}(L[i,k] * C[k,j]) = B[Ip[i],j]$
  $UX = C$, $\text{Sum}\{k \ge i\}(U[i,k] * X[k,j]) = C[i,j]$.

The solution X may overwrite B but not HU.

```
Subroutine  HUXPB( HU, Id, IP, N, B, X, M ):
    Integer values  Id, N, M ;  Integer variable  IP[N+] ;
    Real variables  HU[Id, N+],  B[Id, M+],  X[Id, M+] ;

    Integer  i, j, k, L ;
    Real  z,  C[N+] ;
    Tempreal  tsum,  T[N+] ; ... more precise than Reals. ... *1
    Equivalence  (C,T) ; ... Save storage by packing C inside T .
    Common /L1BWSP/  T ; ... shared workspace.
    Logical UnSav ; ... Gradual Underflow matters only in  X .
```

```
Unsav := UndrflowFlag(.false.) ;

For  j = 1 to M ; ... solve for column  j  :
    for  i = 1 to N ;
        tsum := B[IP[i],j] ;  L := N+1-i ;
        for  k = 1 to i-1  do  tsum := tsum - HU[L+k,L]*C[k] ;
        C[i] := tsum ;                                    ... *2
        next i ;
    for  k = N to 1 step -1  do  T[k] := C[k] ;         ... *3
    for  k = N to 1 step -1 ;
        UnSav := UndrflowFlag(UnSav) ; ... Expose Underflow.
        X[k,j] := z := T[k]/HU[k,k] ;                     ... *4
        UnSav := UndrflowFlag(UnSav) ; ... Hide Underflow.
        for  i = 1 to k-1  do  T[i] := T[i] - HU[i,k]*z ;
        next k ;                                          ... *5
    next j ;
UnSav := UndrflowFlag(UnSav) ; ... Reveal  X 's  Underflows.
return ;
end HUXPB .
```

*Notes: The foregoing code can be modified slightly to give marginally more accurate results at no significant extra cost provided multiplication of Real by Tempreal is only slightly slower than Real by Real. First merge declaration ... *1 with its two neighbors thus:

```
Tempreal z, tsum, T[N+]; ... more precise than Reals. ... 1*
```

Next replace two references to *C*[...] by *T*[...] in statement ... *2 and its predecessor; and delete statement ... *3. Finally, but only if references to UndrflowFlag() cost rather more than a handfull of memory references, replace ... *4 by

```
T[k] := z := T[k]/HU[k,k] ;                              ... 4*
```

and move the adjacent statements to bracket a new statement inserted after ... *5 thus:

```
k;                                                       ... *5

UnSav := UndrflowFlag(UnSav) ; ... Expose Underflow.
for i = 1 to N do X[i,j] := T[i];
UnSav := UndrflowFlag(UnSav) ; ... Hide Underflow.
next j ; ... etc.
```

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Comparison of HU... with LU... :

Programs, like RESYS , that use LUPA and LUXPB can instead use HUPA and HUXPB respectively to get the same results but at different speeds. At first sight, two pairs of programs appear to be under consideration; actually there are three pairs:

LU... accumulating scalar products extra precisely (method 1a).
LU... alternative versions using column-oriented code (1b).
HU... with $L[i,j] = HU[N+1-i+j, N+1-i]$.

The HU... codes should be never much slower than the first LU... codes, and always significantly faster than the second LU... codes, even on vectorized and pipelined parallel machines, unless compiled with an allegedly optimizing compiler that fails to recognize and optimize subscript references of the form $HU[L+k, L]$ when L is fixed and k varies in an inner loop. Here we assume that arrays are stored by columns as prescribed for Fortran.

The extra-precise accumulation of scalar products is a practice in decline on the largest and fastest computers. Part of the decline is attributable to the omission, from the instruction sets of newer machines, of an instruction that evaluates a product to wider precision than the factors; that omission may be motivated by the belief that page faults and similar artifacts of memory management will drive numerical analysts to use column-oriented codes exclusively rather than sacrifice speed to achieve a little more accuracy. The HU... codes sacrifice neither speed nor accuracy, so perhaps the issues should be reconsidered.

Transpositions and Permutations:

There are two ways to keep track of the pivotal exchanges of rows during Gaussian Elimination. One way uses an array $ip[.]$ of n indices $ip[1], ip[2], ..., ip[n]$ to represent the n by n permutation matrix P directly thus:

row $ip[i]$ of A is row i of PA.

Hence, $\{ip[1], ip[2], ..., ip[n]\}$ is a permutation of the indices $\{1, 2, ..., n\}$. The second way represents P as a product of $n-1$ transpositions thus:

$$P = (n-1, k[n-1])(n-2, k[n-2])(...)(3, k[3])(2, k[2])(1, k[1])$$

where each $(i, k[i])$ is a transposition (exchange) of the rows in positions i and $k[i]$; moreover $i \le k[i]$. These indices $k[.]$ are called "imax" in programs LUPA and HUPA , where they are encountered and applied in order $k[1], k[2], k[3], ..., k[n-1]$ to produce the array $ip[.]$ thus:

for $i = 1$ to n do $ip[i] := i$; ... initialization
for $i = 1$ to $n-1$ do swap($ip[i], ip[k[i]]$); ... build $ip[.]$

Given this array $ip[.]$, can we reverse the process to recover the array $k[.]$? Yes. But first the permutation $iq[.]$ inverse to $ip[.]$ must be calculated thus:

for $i = 1$ to n do $iq[ip[i]] := i$; ... inversion.

Now row $iq[i]$ of PA is row i of A. Next we gradually transform $ip[.]$ and $iq[.]$ back to identity permutations while keeping them inverse to each other as $k[.]$ is recovered thus:

for $i = 1$ to $n-1$ do begin
  $k[i] := ip[i]$; ... reversion
  swap($ip[i], ip[iq[i]]$); ... so now $ip[i] = i$
  swap($iq[i], iq[k[i]]$); ... so now $iq[i] = i$
  end ;

One application of the reversion is to reveal the sign of

$\det(A) = \det(PA)/\det(P) = \det(U)/\det(P)$, where
$\det(P) = (-1)^{(\text{number of instances when } k[i]>i)}$.

Another application is to the encoding of P within L to dispense with the bother of providing for the array $IP[.]$ when the factors L and U are saved for subsequent re-use. The encode function $E(x)$ maps the reals x with $|x| \le 1$ to $|E(x)| \ge 2$:

if $x = 0$ then $E(x) :=$ Copysign$(2, x)$ else $E(x) := Scalb(x, K)$

where K is an integer barely large enough that Scalb$(1.0, K)$ overflows to infinity. $K = 128$ for Single, or 1024 for Double precision in the proposed IEEE standard 754. The decode function $D(x)$ inverse to $E(x)$ is

if x is infinite then $D(x) :=$ Copysign$(1, x)$
else if $|x = 2|$ then $D(x) :=$ Copysign$(0, x)$
else $D(x) :=$ Scalb$(x, -K)$; ... and ignore Underflow .

Then to encode $IP[.]$ within L we revert $IP[.]$ to $k[.]$ and then replace $L[k[j], j]$ by $E(L[k[j], j])$ whenever $k[j] > j$. To recover $k[.]$ later, we scan $\{L[i, j], j < i \le n\}$ to find where $|L[k[j], j]| > 1$, thereby determining $k[j] > j$; otherwise $k[j] = j$.

The success of the reversion process above is tantamount to a

Theorem: Every permutation of n positions can be expressed uniquely as a product of $n-1$ transpositions $(n-1, k[n-1])(n-2, k[n-2])(\ldots)(2, k[2])(1, k[1])$ in which each $k[i] \ge i$.

The theorem's validity can be confirmed by running the following program:

```
Program Proof(uptoN):
    procedure Nest(m):
    if m>0 then for j = m to n do begin
                                  k[m] := j ;  Nest(m-1)
                                  end
    else begin
        for i = 1 to n  do  ip[i] := i ;
        for i = 1 to n-1  do  swap( ip[i], ip[k[i]] ) ;
        for i = 1 to n  do  iq[ip[i]] := i ;
        for i = 1 to n-1  do begin
                        if ip[i]=k[i] then begin
                            swap( ip[i], ip[iq[i]] );
                            swap( iq[i], iq[k[i]] )
                            end
```

```
                        else begin
                           write( "Test fails at  n ="; n
                                " with  i = "; i
                                " and  k[.] = "; k[.]
                                "      ip[.] = "; ip[.]
                                "      iq[.] = "; iq };
                           stop
                           end
                        end;
      write( " n = "; n ; " tested successfully." }
      end end Nest ;
   for n = 1 to uptoN  do  Nest(n) ;  write( "End of test.}
   end Proof.
```

Inverting the Hilbert matrix:
Floating-point matrix inversion programs are customarily tested on an $n \times n$ Hilbert matrix H whose elements are $H_{i,j} = 1/(i+j+p-1)$ for $1 \le i, j \le n$ and any integer $p \ge 0$. Because H becomes so ill-conditioned as n or p becomes big, its inverse $W = H^{-1}$ becomes difficult to compute accurately in the face of roundoff. None the less, a way exists to compute W exactly and easily; it uses a little-known formula $W = V\,H\,V$ where V is a diagonal matrix of integers $V_j = (-1)^j((n+j+p-1)!)/((n-j)!(j-1)!(j+p-1)!)$ obtained from a simple recurrence in which only integers appear:

$V_1 := -n$; for $k = 1$ to p do $V_1 := (V_1/k)(n+k)$;
for $j = 1$ to $n-1$ do $V_{j+1} := (((V_j/(j+p))(j-n))/j)(n+j-p)$.

Then $W_{i,j} := V_i V_j/(i+j+p-1)$. (S. Schechter, MTAC, 1959)

Since the elements of H are reciprocals of integers, they cannot be represented exactly in floating-point but must be rounded off. These initial rounding errors may do more damage to H^{-1} than the inversion program under test. To avoid them, we actually use

$$A := mH, \text{ where } m := \text{ LCM}(p+1, p+2, p+3, ..., p+2n-1),$$

which has integer elements all representable exactly in floating-point provided n and p are not too big. Then the inversion program is tested by using it to solve $AX = mI$ numerically for X. Here I is the $n \times n$ identity matrix. Since ideally X should match W, the error introduced by the program under test is indicated by displaying a rough measure of the relative error in X:

$$r = \max_{i,j} |\, X_{i,j} - W_{i,j} \,| \,/\, |\, W_{i,j} \,| \,.$$

This statistic makes no allowance for the ill-condition of H nor for the precision of the arithmetic in which X was calculated. The ill-condition of H can be gauged from

$$c = \max_i \sum_j |\, H_{i,j} W_{i,j} \,| \,.$$

which exceeds 1 to an extent that indicates how severe is cancellation when $HW = I$ is evaluated. The precision is indicated by

u = 1.000...001 - 1.000...000 = 0.000...001
= One unit in the last place carried in numbers near 1.

Then one figure of merit for the program under test is

$$q = r/(uc);$$

the smaller is q, the better the program. Normally $r < 1$ and $q < n$; but when $r > 1$ the matrices A and H are so nearly singular that the program cannot be relied upon to get even one significant digit correct in X, and then the value of q becomes irrelevant. Another figure of merit is the largest value of n for which $r < 1$; the larger is this n, the better.

The error r, and therefore q, depend upon rounding errors that occur during the calculation of X, but rounding errors are not entirely dependable; they behave sometimes almost as if they were random. Therefore prudence demands that roundoff be sampled more than once before conclusions be drawn about a program's vulnerability to roundoff. For instance, most matrix inversion programs, and certainly those using $LUPA$ and $HUPA$ above, will generate different rounding errors if the column ordering of the matrix being inverted is changed. To be more specific, let S be the $n \times n$ permutation matrix that reverses order; that is,

$$S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{when } n = 3.$$

Then the inverse of SHS is SWS, but the computed solution Z of $(SAS)Z = mI$ usually differs from SXS because of differences in the way roundoff occurs. Calculating r and q from Z instead of X gives a second opinion about the effect of roundoff upon the program under test.

To calculate $m = LCM(p+1, p+2, p+3, ..., p+2n-1)$, do thus:

GCD(x, y): while $y \neq 0$ do $\{z := y; y := x \text{ rem } z; x := z\}$;
return GCD := $| x |$ end GCD.

LCM(x, y): if $x = 0$ then return LCM := 0
else return LCM := $(| y | / \text{GCD}(x, y)) * | x |$ end LCM.

$m := p + 1$; for $k = p + 2$ to $p + 2 * n - 1$ do $m := LCM(m, k)$;
... yields m.

For example, when $p = 1$, we find ...

$n = 8$	$n = 9$	$n = 10$ or 11	$n = 12$
$m = 360360$	$m = 12252240$	$m = 232792560$	$m = 5354228880$