LAPACK Working Note 101
A Proposal for a Fortran 90 Interface for LAPACK

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1 Introduction

The purpose of this paper is to initiate discussion of the design of a Fortran 90 interface to LAPACK [1]. Our emphasis at this stage is on the design of an improved *user-interface* to the package, taking advantage of the considerable simplifications which Fortran 90 allows.

The new interface can be implemented initially by writing Fortran 90 jackets to call the existing Fortran 77 code.

Eventually we hope that the LAPACK code will be rewritten to take advantage of the new features of Fortran 90, but this will be an enormous task. We aim to design an interface which can persist unchanged while the underlying code is rewritten.

For convenience we use the name "LAPACK77" to denote the existing Fortran 77 package, and "LAPACK90" to denote the new Fortran 90 interface which we are proposing.

2 LAPACK77 and Fortran 90 Compilers

2.1 Linking LAPACK77 to Fortran 90 programs

LAPACK77 can be called from Fortran 90 programs in its present form — with some qualifications. The qualifications arise only because LAPACK77 is not written entirely in

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standard Fortran 77; the exceptions are the use of the `COMPLEX*16` data type and related intrinsic functions, as listed in Section 6.1 of [1]; these facilities are provided as extensions to the standard language by many Fortran 77 and Fortran 90 compilers. Equivalent facilities are provided in standard Fortran 90, using the parameterized form of the `COMPLEX` data type (see below).

To link LAPACK77 to a Fortran 90 program (which must of course be compiled by a Fortran 90 compiler), one of the following approaches will be necessary, depending on the compilers available.

1. Link the Fortran 90 program to an existing LAPACK77 library, compiled by a Fortran 77 compiler. This approach can only work if the compilers have designed to allow cross-linking.
2. If such cross-linking is not possible, recompile LAPACK77 with the Fortran 90 compiler, provided that the compiler accepts `COMPLEX*16` and related intrinsics as extensions, and create a new library.
3. If these extensions are not accepted, convert the LAPACK77 code to standard Fortran 90 (see below), before recompiling it.

The conversions needed to create standard Fortran 90 code for LAPACK77 are:

`COMPLEX*16`	$\Rightarrow$	`COMPLEX(KIND=Kind(0.0D0)`
`DCONJG(z)` for `COMPLEX*16 z`	$\Rightarrow$	`CONJG(z)`
`DBLE(z)` for `COMPLEX*16 z`	$\Rightarrow$	`REAL(z)`
`DIMAG(z)` for `COMPLEX*16 z`	$\Rightarrow$	`AIMAG(z)`
`DCMPLX(x,y)` for `DOUBLE PRECISION x, y`	$\Rightarrow$	`CMPLX(x,y,KIND=Kind(0.0D0))`

One further obstacle may remain: it is possible that if LAPACK77 has been recompiled with a Fortran 90 compiler, it may not link correctly to an optimized assembly-language BLAS library that has been designed to interface with Fortran 77. Until this is rectified by the vendor of the BLAS library, Fortran 77 code for the BLAS must be used.

2.2 Interface blocks for LAPACK77

Fortran 90 allows one immediate extra benefit to be provided to Fortran 90 users of LAPACK77, without making any further changes to the existing code: that is a *module* of *explicit interfaces* for the routines. If this module is accessed by a `USE` statement in any program unit which makes calls to LAPACK routines, then those calls can be checked by the compiler for errors in the numbers or types of arguments.

The module can be constructed by extracting the necessary specification statements from the Fortran 77 code, as illustrated by the following example (in fixed-form source format) containing an interface for the single routine `CBDSQR`:

```
      MODULE LAPACK77_INTERFACES
```

```
      INTERFACE
      SUBROUTINE CBDSQR( UPLO, N, NCVT, NRU, NCC, D, E, VT, LDVT, U,
     $                   LDU, C, LDC, RWORK, INFO )
      CHARACTER          UPLO
      INTEGER            INFO, LDC, LDU, LDVT, N, NCC, NCVT, NRU
      REAL               D( * ), E( * ), RWORK( * )
      COMPLEX            C( LDC, * ), U( LDU, * ), VT( LDVT, * )
      END
      END INTERFACE
      END MODULE LAPACK77_INTERFACES
```

A single module containing interfaces for all the routines in LAPACK77 (over 1000 of them) may be too large for practical use; it may be desirable to split it (perhaps, one module for single precision documented routines, one for double precision documented routines, and similarly for auxiliary routines).

3 Proposals for the Design of LAPACK90

In the design of a Fortran 90 interface to LAPACK, we propose to take advantage of the features of the language listed below.

1. **Assumed-shape arrays:** All array arguments to LAPACK90 routines will be assumed-shape arrays. Arguments to specify problem-dimensions or array-dimensions will not be required.

   This implies that the actual arguments supplied to LAPACK routines *must* have the *exact* shape required by the problem. The most convenient ways to achieve this are:

   - using allocatable arrays, for example:

     ```
     REAL, ALLOCATABLE :: A(:,:), B(:)
       . . .
     ALLOCATE( A(N,N), B(N) )
       . . .
     CALL LA_GESV( A, B )
     ```

   - passing array sections, for example:

     ```
     REAL :: A(NMAX,NMAX), B(NMAX)
       . . .
     CALL LA_GESV( A(:N,:N), B(:N) )
     ```

   Zero dimensions (empty arrays) will be allowed.

   There are some grounds for concern about the effect of assumed-size arrays on performance, because compilers cannot assume that their storage is contiguous. The effect on performance will of course depend on the compiler, and may diminish in time as compilers become more effective in optimizing compiled code. This point needs investigation.

2. **Automatic allocation of work arrays:** Workspace arguments and arguments to specify their dimensions will not be needed. In simple cases, *automatic arrays* of the required size can be declared internally. In other cases, allocatable arrays may need to be declared and explicitly allocated. Explicit allocation is needed in particular when the amount of workspace required depends on the block-size to be used (which is not passed as an argument).

3. **Optional arguments:** In LAPACK77, character arguments are frequently used to specify some choice of options. In Fortran 90, a choice of options can sometimes be specified naturally by the presence or absence of optional arguments: for example, options to compute the left or right eigenvectors can be specifed by the presence of arguments `VL` or `VR`, and the character arguments `JOBVL` and `JOBVR` which are required in the LAPACK77 routine `DGEEV`, are not needed in LAPACK90.

   In other routines, a character argument to specify options may still be required, but can itself be made optional if there is a natural default value: for example, in `DGESVX` the argument `TRANS` can be made optional, with default value `'N'`.

   Optional arguments can also help to combine two or more routines into one: for example, the functionality provided by the routine `DGECON` can be made acessible by adding an optional argument `RCOND` to `DGETRF`.

4. **Generic Interfaces:** The systematic occurrence in LAPACK of analogous routines for real or complex data, and for single or double precision lends itself well to the definition of generic interfaces, allowing four different routines to be accessed through the same generic name.

   Generic interfaces can also be used to cover routines whose arguments differ in *rank*, and thus provide a slight increase in flexibility over LAPACK77. For example, in LAPACK77, routines for solving a system of linear equations (such as DGESV), allow for multiple right hand sides, and so the arrays which hold the right hand sides and solutions are always of rank 2. In LAPACK90, we can provide alternative versions of the routines (covered by a single generic interface) in which the arrays holding the right hand sides and solutions may *either* be of rank 1 (for a single right hand side) *or* be of rank 2 (for several right hand sides).

5. **Naming:** For the generic routine names, we propose:

   (a) the initial letter (`S`, `C`, `D` or `Z`) is simply omitted.

   (b) the letters `LA_` are prefixed to all names to identify them as names of LAPACK routines.

   In other respects the naming scheme remains the same as described in Section 2.1.3 of [1]: for example, `LA_GESV`.

   It would also be possible to define longer, more meaningful names (which could co-exist with the shorter names), but we have not attempted this here.

   We have *not* proposed the use of any *derived types* in this Fortran 90 interface. They could be considered — for example, to hold the details of an *LU* factorization and equilibration factors. However, since LAPACK routines are so frequently used as building blocks in larger algorithms or applications, we feel that there are advantages in keeping the interface simple, and avoiding possible loss of efficiency through the use of array pointers (which such derived types would require).

6. **Error-handling:**

   In LAPACK77, all documented routines have a diagnostic output argument `INFO`. Three types of exit from a routine are allowed:

   successful termination: the routine returns to the calling program with `INFO` set to 0.

   illegal value of one or more arguments: the routine sets `INFO`< 0 and calls the auxiliary routine `XERBLA`; the standard version of XERBLA issues an error message identifying the first invalid argument, and stops execution.

   failure in the course of computation: the routine sets `INFO` > 0 and returns to the calling program without issuing any error message. Only some LAPACK77 routines need to allow this type of error-exit; it is then the resposibility of a user to test `INFO` on return to the calling program.

   For LAPACK90 we propose that the argument `INFO` becomes *optional*: if it is not present and an error occurs, then the routine *always* issues an error message and stops execution, even when `INFO`> 0 (in which case the error message reports the value of `INFO`). If a user wishes to continue execution after a failure in computation, then `INFO` must be supplied and tested on return.

   This behaviour simplifies calls to LAPACK90 routines when there is no need to test `INFO` on return, and makes it less likely that users will forget to test `INFO` when necessary.

   If an invalid argument is detected, we propose that routines issue an error message and stop, as in LAPACK77. Note however that in Fortran 90 there can be different reasons for an argument being invalid:

   illegal value : as in LAPACK77.

   invalid shape (of an assumed-shape array): for example, a 2-dimensional array is not square when it is required to be.

   inconsistent shapes (of two or more assumed-shape arrays): for example, arrays holding the right hand sides and solutions of a system of linear equations must have the same shape.

   The specification could be extended so that the error-message could distinguish between these cases.

4 Prototype Implementation of LAPACK90 Procedures

We have implemented Fortran 90 jacket procedures to the group of LAPACK77 routines concerned with the solution of systems of linear equations $AX = B$ for a general matrix A — that is, the driver routines `xGESV` and `xGESVX`, and the computational routines `xGETRF`, `xGETRS`, `xGETRI`, `xGECON`, `xGERFS` and `xGEEQU`.

In Appendix A, we give detailed documentation of the proposed interfaces. Here we give examples of calls to each of the proposed routines, the first without using any of the optional arguments, the second using all the arguments. For the time being and for ease of comparison between LAPACK77 and LAPACK90, we have retained the same names for the corresponding arguments, although of course Fortran 90 offers the possibility of longer names (for example, `IPIV` could become `PIVOT_INDICES`).

In this prototype implementation, we have assumed that the code of LAPACK77 is not modified.

`LA_GESV` (simple driver):

```
CALL LA_GESV( A, B )

CALL LA_GESV( A, B, IPIV, INFO )
```

Comments:

- The array `B` may have rank 1 (one right hand side) or rank 2 (several right hand sides).

`LA_GESVX` (expert driver):

```
CALL LA_GESVX( A, B, X )

CALL LA_GESVX( A, B, X, AF, IPIV, FACT, TRANS, EQUED, R, C, &
               FERR, BERR, RCOND, RPVGRW, INFO )
```

Comments:

- The arrays `B` and `X` may have rank 1 (in which case `FERR` and `BERR` are scalars) or rank 2 (in which case `FERR` and `BERR` are rank-1 arrays).
- `RPVGRW` returns the reciprocal pivot growth factor (returned in `WORK(1)` in LAPACK77).
- the presence or absence of `EQUED` is used to specify whether or not equilibration is to be performed, instead of the option `FACT = 'E'`.

`LA_GETRF` (LU factorization):

```
CALL LA_GETRF( A, IPIV )

CALL LA_GETRF( A, IPIV, RCOND, NORM, INFO )
```

Comments:

- instead of a separate routine `LA_GECON`, we propose that optional arguments `RCOND` and `NORM` are added to `LA_GETRF` to provide the same functionality in a more convenient manner. The argument `ANORM` of `xGECON` is not needed, because `LA_GETRF` can always compute the norm of A if required.

LA_GETRS (solution of equations using LU factorization):

```
CALL LA_GETRS( A, IPIV, B )

CALL LA_GETRS( A, IPIV, B, TRANS, INFO )
```

Comments:

- The array B may have rank 1 or 2.

LA_GETRI (matrix inversion using LU factorization):

```
CALL LA_GETRI( A, IPIV )

CALL LA_GETRI( A, IPIV, INFO )
```

LA_GERFS (refine solution of equations and optionally compute error bounds):

```
CALL LA_GERFS( A, AF, IPIV, B, X )

CALL LA_GERFS( A, AF, IPIV, B, X, TRANS, FERR, BERR, INFO )
```

Comments:

- The arrays B and X may have rank 1 (in which case FERR and BERR are scalars) or rank 2 (in which case FERR and BERR are rank-1 arrays).

LA_GEEQU (equilibration):

```
CALL LA_GEEQU( A, R, C )

CALL LA_GEEQU( A, R, C, ROWCND, COLCND, AMAX, INFO )
```

5 Documentation

In Appendix A, we give a first attempt at draft documentation for these routines. The style is somewhat similar to that of the LAPACK Users' Guide, but with various obvious new conventions introduced to handle the generic nature of the interfaces.

6 Test Software

Additional test software will be needed to test the new interfaces.

7 Timings

We have done some timings to measure the extra overhead of the Fortran 90 interface. We timed **LA_GETRF** on a single processor of an IBM SP-2 (in double precision) and a single processor of a Cray YMP C92 (in single precision). All timings are given in megaflops.

IBM 1. Speed of LAPACK90 calling LAPACK77 and BLAS from the ESSL library.

2. Speed of LAPACK77, using BLAS from the ESSL library.

Array size	600	700	800	900	1000	1100	1200	1300	1400	1500
LAPACK90	187	180	182	170	172	172	176	177	181	182
LAPACK77	191	181	182	171	172	173	176	179	180	182

Cray 1. speed of LAPACK90 calling LAPACK77 as provided by CRAY in LIBSCI.

2. Speed of LAPACK77 as provided by CRAY in LIBSCI.

Array size	600	700	800	900	1000	1100	1200	1300	1400	1500
LAPACK90	260	781	260	812	266	832	268	847	270	856
LAPACK77	261	787	261	817	267	838	268	851	271	859

Two conclusion can be taken from the above tables:

1. The LAPACK90 results can be a little slower (1 or 2%) than the LAPACK77 results.
2. The Cray timings show a striking loss of speed for matrix sizes which are a multiple of 8. In these tests, the leading dimension of the array holding the matrix was equal to the matrix size (as naturally happens when using assumed-shape arrays); when the leading dimension is a multiple of 8, memory bank conflicts slow the computations down. A more careful implementation of the BLAS might be able to reduce this sensitivity to the value of the leading dimension. In Fortran 77, a user can always avoid the problem by declaring arrays with odd values for the leading dimension. In Fortran 90, the situation is more complicated; with the current implementation of LAPACK90, it is likely that the compiler will pass a temporary copy of the array A (with leading dimension N) to the LAPACK77 code where all the intensive work is done – so users would have no means of avoiding memory bank conflict in the LAPACK77 code. If Fortran 90 code were used throughout then assumed-shape arrays could be used everywhere and the compiler sould not need to create any temporary copies, and users would have more control.

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References

[1] E. Anderson, Z. Bai, C. H. Bischof, J. Demmel, J. J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov, and D. C. Sorensen. *LAPACK Users' Guide Release 2.0*. SIAM, Philadelphia, 1995.

[2] M. Metcalf and J. Reid *Fortran 90 Explained.* Oxford, New York, Tokyo, Oxford University Press, 1990.

A Documentation of LAPACK90 Procedures

A.1 LA_GESV

A.1.1 Purpose

LA_GESV computes the solution to either a real or complex system of linear equations $AX = B$, where A is a square matrix and B and X are either rectangular matrices or vectors.

The LU decomposition with partial pivoting and row interchanges is used to factor A as $A = PLU$, where P is a permutation matrix, L is unit lower triangular, and U is upper triangular. The factored form of A is then used to solve the system of equations $AX = B$.

A.1.2 Specification

SUBROUTINE LA_GESV(A, B, IPIV, INFO)
    type(*wp*), INTENT(INOUT) :: A(:,:), *rhs*
    INTEGER, INTENT(OUT), OPTIONAL :: IPIV(:)
    INTEGER, INTENT(OUT), OPTIONAL :: INFO
    where
    type ::= REAL | COMPLEX
    wp ::= KIND(1.0) | KIND(1.0D0)
    rhs ::= B(:,:) | B(:)

A.1.3 Arguments

A – (*input/output*) either **REAL** or **COMPLEX** square array, shape $(:,:)$, $size(A,1) = size(A,2)$.

- On entry, the matrix A.
- On exit, the factors L and U from the factorization $A = PLU$; the unit diagonal elements of L are not stored.

B – (*input/output*) either **REAL** or **COMPLEX** rectangular array, shape either $(:,:)$ or $(:)$, $size(B,1)$ or $size(B) = size(A,1)$.

- On entry, the right hand side vector(s) of matrix B for the system of equations $AX = B$.
- On exit, if there is no error, the matrix of solution vector(s) X.

IPIV – *Optional* (*output*) **INTEGER** array, shape $(:)$, $size(IPIV) = size(A,1)$. If $IPIV$ is present, it contains indices that define the permutation matrix P; row i of the matrix was interchanged with row $IPIV(i)$.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present

$= 0$: successful exit

< 0 : if $INFO = -i$, the i-th argument had an illegal value

≥ 0 : if $INFO = k$, $U(k,k)$ is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.

- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.2 LA_GESVX

A.2.1 Purpose

LA_GESVX computes the solution to a either real or complex system of linear equations $AX = B$, where A is a square matrix and B and X are either rectangular matrices or vectors.

LA_GESVX is an expert driver routine, which can also optionally perform the following functions:

- solve $A^T X = B$ or $A^H X = B$,
- estimate the condition number of A
- return the pivot growth factor
- refine the solution and compute forward and backward error bounds
- equilibrate the system if A is poorly scaled.

A.2.2 Specification

```
SUBROUTINE LA_GESVX (A, B, X, AF, IPIV, FACT, TRANS, &
       EQUED, R, C, FERR, BERR, RCOND, RPVGRW, INFO)
   type(wp), INTENT(INOUT) :: A(:,:), rhs
   type(wp), INTENT(OUT) :: sol
   type(wp), INTENT(INOUT), OPTIONAL :: AF(:,:)
   INTEGER, INTENT(INOUT), OPTIONAL :: IPIV(:)
   CHARACTER(LEN=1), INTENT(IN), OPTIONAL :: FACT, &
         TRANS
   CHARACTER(LEN=1), INTENT(INOUT), OPTIONAL :: &
         EQUED
   REAL(wp), INTENT(INOUT), OPTIONAL :: R(:), C(:)
   REAL(wp), INTENT(OUT), OPTIONAL :: err, RCOND, &
         RPVGRW
   INTEGER, INTENT(OUT), OPTIONAL :: INFO
   where
   type ::= REAL | COMPLEX
   wp ::= KIND(1.0) | KIND(1.0D0)
   rhs ::= B(:,:) | B(:)
   sol ::= X(:,:) | X(:)
   err ::= FERR(:), BERR(:) | FERR, BERR
```

A.2.3 Description

The following steps are performed:

1. If $FACT$ is not present or $FACT = 'N'$, and $EQUED$ is present, real scaling factors are computed to equilibrate the system:

   TRANS = 'N' : $diag(R)\ A\ diag(C)\ (diag(C))^{-1}\ X = diag(R)\ B$

   TRANS = 'T' : $(diag(R)\ A\ diag(C))^T\ (diag(R))^{-1}\ X = diag(C)\ B$

   TRANS = 'C' : $(diag(R)\ A\ diag(C))^H\ (diag(R))^{-1}\ X = diag(C)\ B$

   Whether or not the system will be equilibrated depends on the scaling of the matrix A, but if equilibration is used, A is overwritten by $diag(R)\ A\ diag(C)$ and B by $diag(R)\ B$ (if $TRANS = 'N'$) or $diag(C)\ B$ (if $TRANS = 'T'$ or $'C'$).

2. If $FACT = 'N'$, the LU decomposition is used to factor the matrix A (after equilibration if $EQUED$ is present) as $A = PLU$, where P is a permutation matrix, L is a unit lower triangular matrix, and U is upper triangular.

3. The factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than machine precision, steps $4 - 6$ are skipped.

4. The system of equations is solved for X using the factored form of A.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by $diag(C)$ (if $TRANS = 'N'$) or $diag(R)$ (if $TRANS = 'T'$ or $'C'$) so that it solves the original system before equilibration.

A.2.4 Arguments

A – (*input/output*) either **REAL** or **COMPLEX** square array, shape $(:,:)$, $size(A,1) = size(A,2)$.

If $FACT$ is not present or $FACT = 'N'$,

- On entry, the matrix A.
- On exit, if $EQUED$ is present, the matrix A may have been overwritten by the equilibrated matrix (see $EQUED$).

If $FACT$ is present and $FACT = 'F'$,

- On entry, the matrix A, possibly equilibrated in a previous call to **LA_GESVX** (see $EQUED$).
- On exit, A is unchanged.

B – (*input/output*) either **REAL** or **COMPLEX** rectangular array, shape either $(:,:)$ or $(:)$, $size(B,1)$ or $size(B) = size(A,1)$.

- On entry, the right hand side vector(s) of matrix B for the system of equations $AX = B$.
- On exit, if $EQUED$ is present, B may have been scaled in accordance with the equilibration of A (see $EQUED$); otherwise, B is unchanged.

X – (*output*) either **REAL** or **COMPLEX** rectangular array, shape either $(:,:)$ or $(:)$, $size(X,1)$ or $size(X) = size(A,1)$. If $INFO = 0$, the solution matrix (vector) X to the original system of equations. Note that X always returns the solution to the *original* system of equations; if equilibration has been performed ($EQUED$ is present and $EQUED \neq 'N'$), this does not correspond to the scaled A and B.

AF – *Optional* (*input/output*) either **REAL** or **COMPLEX** square array, shape $(:,:)$, $size(AF,1) = size(AF,2) = size(A,1)$.

If $FACT$ is not present or $FACT = 'N'$, then AF is an *output* argument and returns the factors L and U from the factorization $A = PLU$ of the original matrix A, possibly equilibrated if $EQUED$ is present.

If $FACT$ is present and $FACT = 'F'$, then AF is an *input* argument (and must be present); on entry, it must contain the factors L and U of A (possibly equilibrated if $EQUED$ is present), returned by a previous call to **LA_GESVX**.

IPIV – *Optional* (*input/output*) **INTEGER** array, shape $(:)$, $size(IPIV) = size(A,1)$.

If $FACT$ is not present or $FACT = 'N'$, then $IPIV$ is an *output* argument and returns the pivot indices from the factorization $A = PLU$ of the original matrix A, possibly equilibrated if $EQUED$ is present.

If $FACT$ is present and $FACT = 'F'$, then $IPIV$ is an *input* argument (and must be present); on entry, it must contain the pivot indices from the factorization of A (possibly equilibrated if $EQUED$ is present), returned by a previous call to **LA_GESVX**.

TRANS – *Optional* (*input*) **CHARACTER*1**.

- If $TRANS$ is present, it specifies the form of the system of equations:

  $= 'N'$: $AX = B$ (No transpose)

  $= 'T'$: $A^T X = B$ (Transpose)

  $= 'C'$: $A^H X = B$ (Conjugate transpose)
- otherwise $TRANS = 'N'$ is assumed.

FACT – *Optional* (*input*) **CHARACTER*1**. Specifies whether or not the factored form of the matrix A is supplied on entry.

- If FACT is present then:

  $= 'N'$: the matrix A will be equilibrated if $EQUED$ is present, then copied to AF and factored.

  $= 'F'$: on entry, AF and $IPIV$ must contain the factored form of A (possibly equilibrated if $EQUED$ is present).
- otherwise $FACT = 'N'$ is assumed.

EQUED – *Optional* (*input/output*) **CHARACTER*1**.

If $FACT$ is not present or $FACT = 'N'$, then $EQUED$ is an *output* argument. If it is present, then the matrix is equilibrated, and on exit $EQUED$ specifies the scaling of A which has actually been performed:

$= 'N'$: No equilibration.

$= 'R'$: Row equilibration, i.e., A has been premultiplied by $diag(R)$; also B has been premultiplied by $diag(R)$ if $TRANS = 'N'$.

$= 'C'$: Column equilibration, i.e., A has been postmultiplied by $diag(C)$; also B has been premultiplied by $diag(C)$ if $TRANS = 'T'$ or $'C'$.

$= 'B'$: Both row and column equilibration: combines the effects of $EQUED = 'R'$ and $EQUED = 'C'$.

If $FACT$ is present and $FACT = 'F'$, then $EQUED$ is an *input* argument; if it is present, it specifies the equilibration of A which was performed in a previous call to **LA_GESVX** with $FACT$ not present or $FACT = 'N'$.

R – *Optional* (*input/output*) **REAL** array, shape (:), $size(R) = size(A, 1)$. R must be present if $EQUED$ is present and $EQUED = 'R'$ or $'B'$; R is not referenced if $EQUED = 'N'$ or $'C'$.

If $FACT$ is not present or $FACT = 'N'$, then R is an *output* argument. If $EQUED = 'R'$ or $'B'$, R returns the row scale factors for equilibrating A.

If $FACT$ is present and $FACT = 'F'$, then R is an *input* argument. If $EQUED = 'R'$ or $'B'$, R must contain the row scale factors for equilibrating A, returned by a previous call to **LA_GESVX**; each element of R must be positive.

C – *Optional* (*input/output*) **REAL** array, shape (:), $size(C) = size(A, 1)$. C must be present if $EQUED$ is present and $EQUED = 'C'$ or $'B'$; R is not referenced if $EQUED = 'N'$ or $'R'$.

If $FACT$ is not present or $FACT = 'N'$, then C is an *output* argument. If $EQUED = 'C'$ or $'B'$, C returns the column scale factors for equilibrating A.

If $FACT$ is present and $FACT = 'F'$, then C is an *input* argument. If $EQUED = 'C'$ or $'B'$, C must contain the column scale factors for equilibrating A, returned by a previous call to **LA_GESVX**; each element of C must be positive.

FERR – *Optional* (*output*) either **REAL** array of shape (:) or **REAL** scalar. If it is an array, $size(FERR) = size(X, 2)$. The estimated forward error bound for each solution vector $X(j)$ (the j-th column of the solution matrix X). If $XTRUE$ is the true solution corresponding to $X(j)$, $FERR(j)$ is an estimated upper bound for the magnitude of the largest element in $(X(j) - XTRUE)$ divided by the magnitude of the largest element in $X(j)$. The estimate is as reliable as the estimate for $RCOND$, and is almost always a slight overestimate of the true error.

BERR – *Optional* (*output*) either **REAL** array of shape (:) or **REAL** scalar. If it is an array, $size(BERR) = size(X, 2)$. The componentwise relative backward error of each solution vector $X(j)$ (i.e., the smallest relative change in any element of A or B that makes $X(j)$ an exact solution).

RCOND – *Optional* (*output*) **REAL**. The estimate of the reciprocal condition number of the matrix A after equilibration (if done). If $RCOND$ is less than the machine precision (in particular, if $RCOND = 0$), the matrix is singular to working precision. This condition is indicated by a return code of $INFO > 0$, and the solution and error bounds are not computed.

RPVGRW – *Optional* (*output*) **REAL**. The reciprocal pivot growth factor $\|A\|_\infty / \|U\|_\infty$. If $RPVGRW$ is much less than 1, then the stability of the LU factorization of the (equilibrated) matrix A could be poor. This also means that the solution X, condition estimator $RCOND$, and forward error bound $FERR$ could be unreliable. If factorization fails with $0 < INFO \le size(A, 1)$, then $RPVGRW$ contains the reciprocal pivot growth factor for the leading $INFO$ columns of A.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present
  - $= 0$: successful exit
  - < 0 : if $INFO = -i$, the i-th argument had an illegal value
  - > 0 : if $INFO = i$, and i is
    - $\le N$: $U(i, i)$ is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution and error bounds could not be computed.
    - $= N + 1$: $RCOND$ is less than machine precision. The factorization has been completed, but the matrix is singular to working precision, and the solution and error bounds have not been computed.
- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.3 LA_GETRF

A.3.1 Purpose

LA_GETRF computes an LU factorization of a general rectangular matrix A using partial pivoting with row interchanges.

The factorization has the form $A = PLU$ where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if $m > n$), and U is upper triangular (upper trapezoidal if $m < n$), where $m = size(A,1)$ and $n = size(A,2)$.

When A is square ($m = n$), **LA_GETRF** optionally estimates the reciprocal of the condition number of the matrix A, in either the 1-norm or the ∞-norm. An estimate is obtained for $\|A^{-1}\|$, and the reciprocal of the condition number is computed as $RCOND = 1/(\|A\|\,\|A^{-1}\|)$.

A.3.2 Specification

SUBROUTINE LA_GETRF(A, IPIV, RCOND, NORM, INFO)
 type(*wp*), INTENT(INOUT) :: A(:,:)
 INTEGER, INTENT(OUT) :: IPIV(:)
 CHARACTER(LEN=1), INTENT(IN), OPTIONAL :: NORM
 REAL(*wp*), INTENT(OUT), OPTIONAL :: RCOND
 INTEGER, INTENT(OUT), OPTIONAL :: INFO
 where
 type ::= REAL | COMPLEX
 wp ::= KIND(1.0) | KIND(1.0D0)

A.3.3 Arguments

A – (*input/output*) either **REAL** or **COMPLEX** array, shape $(:,:)$.

- On entry, the matrix A.
- On exit, the factors L and U from the factorization $A = PLU$; the unit diagonal elements of L are not stored.

IPIV – (*output*) **INTEGER** array, shape (:), $size(IPIV) = \min(size(A,1), size(A,2))$. Indices that define the permutation matrix P; row i of the matrix was interchanged with row $IPIV(i)$.

RCOND – *Optional* (*output*) **REAL**. The reciprocal of the condition number of the matrix A for the case $m = n$, computed as $RCOND = 1/(\|A\|\,\|A^{-1}\|)$. $RCOND$ should be present if $NORM$ is present. If $m \neq n$ then $RCOND$ is returned as zero.

NORM – *Optional* (*input*) **CHARACTER*1**. Specifies whether the 1-norm condition number or the ∞-norm condition number is required:

- = '1', '*O*' or '*o*': 1-norm;
- = '*I*', '*i*': ∞-norm.

If $NORM$ is not present, the 1-norm is used.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present
  $= 0$: successful exit
  < 0 : if $INFO = -k$, the k-th argument had an illegal value
  > 0 :
  if $INFO = k$, $U(k,k)$ is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.
- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.4 LA_GETRS

A.4.1 Purpose

LA_GETRS solves a system of linear equations $AX = B$, $A^TX = B$ or $A^HX = B$ with a general square matrix A, using the LU factorization computed by **LA_GETRF**.

A.4.2 Specification

SUBROUTINE LA_GETRS (A, IPIV, B, TRANS, INFO)
type(*wp*), INTENT(IN) :: A(:,:)
INTEGER, INTENT(IN) :: IPIV(:)
type(*wp*), INTENT(INOUT) :: *rhs*
CHARACTER(LEN=1), INTENT(IN), OPTIONAL :: TRANS
INTEGER, INTENT(OUT), OPTIONAL :: INFO
where
type ::= REAL | COMPLEX
wp ::= KIND(1.0) | KIND(1.0D0)
rhs ::= B(:,:) | B(:)

A.4.3 Arguments

A – (*input*) either **REAL** or **COMPLEX** square array, shape $(:,:)$, $size(A,1) = size(A,2)$. The factors L and U from the factorization $A = PLU$ as computed by **LA_GETRF**.

IPIV – (*input*) **INTEGER** array, shape $(:)$, $size(IPIV) = size(A,1)$. The pivot indices from **LA_GETRF**; for $1 \le i \le size(A,1)$, row i of the matrix was interchanged with row $IPIV(i)$.

B – (*input/output*) either **REAL** or **COMPLEX** rectangular array, shape either $(:,:)$ or $(:)$, $size(B,1)$ or $size(B) = size(A,1)$.

- On entry, the right hand side vector(s) of matrix B for the system of equations $AX = B$.
- On exit, if there is no error, the matrix of solution vector(s) X.

TRANS – *Optional* (*input*) **CHARACTER*1**.

- If $TRANS$ is present, it specifies the form of the system of equations:
  $= 'N'$: $AX = B$ (No transpose)
  $= 'T'$: $A^TX = B$ (Transpose)
  $= 'C'$: $A^HX = B$ (Conjugate transpose)
- otherwise $TRANS = 'N'$ is assumed.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present
  $= 0$: successful exit
  < 0 : if $INFO = -k$, the k-th argument had an illegal value
- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.5 LA_GETRI

A.5.1 Purpose

LA_GETRI computes the inverse of a matrix using the LU factorization computed by **LA_GETRF**.

A.5.2 Specification

SUBROUTINE LA_GETRI (A, IPIV, INFO)
    type(*wp*), INTENT(INOUT) :: A(:,:)
    INTEGER, INTENT(IN) :: IPIV(:)
    INTEGER, INTENT(OUT), OPTIONAL :: INFO
    where
    type ::= REAL | COMPLEX
    wp ::= KIND(1.0) | KIND(1.0D0)

A.5.3 Arguments

A – (*input/output*) either **REAL** or **COMPLEX** square array, shape $(:,:)$, $size(A,1) = size(A,2)$.

- On entry contains the factors L and U from the factorization $A = PLU$ as computed by **LA_GETRF**.
- On exit, if $INFO = 0$, the inverse of the original matrix A.

IPIV – (*input*) **INTEGER** array, shape (:), $size(IPIV) = size(A, 1)$. The pivot indices from **LA_GETRF**; for $1 \le i \le size(A, 1)$, row i of the matrix was interchanged with row $IPIV(i)$.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present
  $= 0$: successful exit
  < 0 : if $INFO = -k$, the k-th argument had an illegal value
  > 0 : if $INFO = k$, U(K,K) is exactly zero; the matrix is singular and its inverse could not be computed.
- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.6 LA_GERFS

A.6.1 Purpose

LA_GERFS improves the computed solution X of a system of linear equations $AX = B$ or $A^T X = B$ and provides error bounds and backward error estimates for the solution. **LA_GERFS** uses the LU factors computed by **LA_GETRF**.

A.6.2 Specification

```
SUBROUTINE LA_GERFS (A, AF, IPIV, B, X, &
      TRANS, FERR, BERR, INFO)
   type(wp), INTENT(IN) :: A(:,:), AF(:,:), rhs
   INTEGER, INTENT(IN) :: IPIV(:)
   type(wp), INTENT(INOUT) :: sol
   CHARACTER(LEN=1), INTENT(IN), OPTIONAL :: TRANS
   REAL(wp), INTENT(OUT), OPTIONAL :: err
   INTEGER, INTENT(OUT), OPTIONAL :: INFO
   where
   type ::= REAL | COMPLEX
   wp ::= KIND(1.0) | KIND(1.0D0)
   rhs ::= B(:,:) | B(:)
   sol ::= X(:,:) | X(:)
   err ::= FERR(:), BERR(:) | FERR, BERR
```

A.6.3 Arguments

A – (*input*) either **REAL** or **COMPLEX** square array, shape $(:, :)$, $size(A, 1) = size(A, 2)$. The original matrix A.

AF – (*input*) either **REAL** or **COMPLEX** square array, shape $(:, :)$, $size(AF, 1) = size(AF, 2) = size(A, 1)$. The factors L and U from the factorization $A = PLU$ as computed by **LA_GETRF**.

IPIV – (*input*) **INTEGER** array, shape (:), $size(IPIV) = size(A, 1)$. The pivot indices from **LA_GETRF**; for $1 \leq i \leq size(A, 1)$, row i of the matrix was interchanged with row $IPIV(i)$.

B – (*input*) either **REAL** or **COMPLEX** rectangular array, shape either (:,:) or (:), $size(B, 1)$ or $size(B) = size(A, 1)$. The right hand side vector(s) of matrix B for the system of equations $AX = B$.

X – (*input/output*) either **REAL** or **COMPLEX** rectangular array, shape either (:,:) or (:), $size(X, 1)$ or $size(X) = size(A, 1)$.

- On entry, the solution matrix X, as computed by **LA_GETRS**.
- On exit, the improved solution matrix X.

TRANS – *Optional* (*input*) **CHARACTER*1**.

- If $TRANS$ is present, it specifies the form of the system of equations:
  $= 'N'$: $AX = B$ (No transpose)
  $= 'T'$: $A^T X = B$ (Transpose)
  $= 'C'$: $A^H X = B$ (Conjugate transpose)
- otherwise $TRANS = 'N'$ is assumed.

FERR – *Optional* (*output*) either **REAL** array of shape (:) or **REAL** scalar. If it is an array, $size(FERR) = size(X, 2)$. The estimated forward error bound for each solution vector $X(j)$ (the j-th column of the solution matrix X). If $XTRUE$ is the true solution corresponding to $X(j)$, $FERR(j)$ is an estimated upper bound for the magnitude of the largest element in $(X(j) - XTRUE)$ divided by the magnitude of the largest element in $X(j)$. The estimate is as reliable as the estimate for $RCOND$, and is almost always a slight overestimate of the true error.

BERR – *Optional* (*output*) either **REAL** array of shape (:) or **REAL** scalar. If it is an array, $size(BERR) = size(X, 2)$. The componentwise relative backward error of each solution vector $X(j)$ (i.e., the smallest relative change in any element of A or B that makes $X(j)$ an exact solution).

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present
  $= 0$: successful exit
  < 0 : if $INFO = -i$, the i-th argument had an illegal value
- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

A.6.4 Internal Parameters

ITMAX – is the maximum number of steps of iterative refinement. It is set to 5 in the **LAPACK77** subroutines (see [1]).

A.7 LA_GEEQU

A.7.1 Purpose

LA_GEEQU computes row and column scalings intended to equilibrate a rectangle matrix A and reduce its condition number. R returns the row scale factors and C the column scale factors, chosen to try to make the largest entry in each row and column of the matrix B with elements $B_{ij} = R_i A_{ij} C_j$ have absolute value 1.

R_i and C_j are restricted to be between $SMLNUM$ = smallest safe number and $BIGNUM$ = largest safe number. Use of these scaling factors is not guaranteed to reduce the condition number of A but works well in practice.

A.7.2 Specification

```
SUBROUTINE LA_GEEQU ( A, R, C, ROWCND, COLCND, &
      AMAX, INFO )
   type(wp), INTENT(IN) :: A(:,:)
   REAL(wp), INTENT(OUT) :: R(:), C(:)
   REAL(wp), INTENT(OUT), OPTIONAL :: ROWCND, &
         COLCND, AMAX
   INTEGER, INTENT(OUT), OPTIONAL :: INFO
   where
   type ::= REAL | COMPLEX
   wp ::= KIND(1.0) | KIND(1.0D0)
```

A.7.3 Arguments

A – (*input*) either **REAL** or **COMPLEX** array, shape $(:,:)$. The matrix A, whose equilibration factors are to be computed.

R – (*output*) **REAL** array, shape $(:)$, $size(R) = size(A,1)$. If $INFO = 0$ or $INFO > size(A,1)$, R contains the row scale factors for A.

C – (*output*) **REAL** array, shape $(:)$, $size(C) = size(A,2)$. If $INFO = 0$, C contains the column scale factors for A.

ROWCND – *Optional* (*output*) **REAL**. If $INFO = 0$ or $INFO > size(A,1)$, $ROWCND$ contains the ratio of the smallest $R(i)$ to the largest $R(i)$. If $ROWCND \geq 0.1$ and $AMAX$ is neither too large nor too small, it is not worth scaling by R.

COLCND – *Optional* (*output*) **REAL**. If $INFO = 0$, $COLCND$ contains the ratio of the smallest $C(i)$ to the largest $C(i)$. If $COLCND \geq 0.1$, it is not worth scaling by C.

AMAX – *Optional* (*output*) **REAL**. Absolute value of largest matrix element. If $AMAX$ is very close to overflow or very close to underflow, the matrix should be scaled.

INFO – *Optional* (*output*) **INTEGER**.

- If $INFO$ is present

  $= 0$: successful exit

  < 0 : if $INFO = -i$, the i-th argument had an illegal value

  > 0 : if $INFO = i$, and i is

    $\leq m$: the i-th row of A is exactly zero

    $> m$: the $(i - m)$-th column of A is exactly zero

    where $m = size(A, 1)$.

- If $INFO$ is not present and an error occurs, then the program is terminated with an error message.

B Code for One Version of LA_GESV

We illustrate here the sort of code that is needed to implement one of the Fortran 90 jacket procedures. The procedure shown is the real single precision version of **LA_GESV**, with multiple right hand sides (B is a rank-2 array).

B.1 Precision-dependencies

To handle different precisions, we use a module LA_PRECISION to define named constants SP and DP for the kind values of single and double precision, respectively.

```
MODULE LA_PRECISION
  INTEGER, PARAMETER :: SP=KIND(1.0), DP=KIND(1.0D0)
END MODULE LA_PRECISION
```

Within the LAPACK90 code, all real and complex constructs are expressed in terms of a symbolic kind value WP, which is defined by reference to the module LA_PRECISION — in single precision:

```
USE LA_PRECISION :: WP => SP
```

and in double precision:

```
USE LA_PRECISION :: WP => DP
```

These are the only precision-dependent changes in the code, apart from changes to the procedure-names.

B.2 Error-handling

To handle errors, as described in Section 4, we use a simple procedure ERINFO, which is assumed to be accessed from a module LA_AUX:

```
SUBROUTINE ERINFO(LINFO, SRNAME, INFO)
!  .. Scalar Arguments ..
   CHARACTER( LEN = * ), INTENT(IN) :: SRNAME
   INTEGER             , INTENT(IN) :: LINFO
   INTEGER             , INTENT(INOUT), OPTIONAL :: INFO
!
!  .. Executable Statements ..
!
   IF( PRESENT(INFO) ) INFO = LINFO
   IF( LINFO < 0 .OR. LINFO>0 .AND. .NOT.PRESENT(INFO) )THEN
```

```
        WRITE (*,*) 'Program terminated in LAPACK_90 subroutine ', SRNAME
        WRITE (*,*) 'Error indicator, INFO = ', LINFO
        STOP
     END IF
  END SUBROUTINE ERINFO
```

A more elaborate error-handling mechanism could of course be devised.

B.3 Accessing LAPACK77 routines

We assume that interface-blocks for all the LAPACK77 routines are accessible from a module `LAPACK77_INTERFACES`. Note that we do not use generic interfaces for the LAPACK77 routines, since that would impose some restrictions on the way in which LAPACK77 routines could be called.

However, we rename the routine in the `USE` statement, so that the precision-dependent name-change is localized in the `USE` statement.

B.4 The code

```
   SUBROUTINE SGESV_F90(A,B,IPIV,INFO)
!     .. Use Statements ..
      USE LA_PRECISION, ONLY: WP => SP
      USE LA_AUX, ONLY: ERINFO
      USE LAPACK77_INTERFACES, ONLY: GESV_F77 => SGESV
!     .. Implicit Statement ..
      IMPLICIT NONE
!     .. Scalar Arguments ..
      INTEGER, INTENT(OUT), OPTIONAL :: INFO
!     .. Array Arguments ..
      INTEGER, INTENT(OUT), OPTIONAL, TARGET :: IPIV(:)
      REAL(WP), INTENT(INOUT) :: A(:,:), B(:,:)
!     .. Parameters ..
      CHARACTER(LEN=7), PARAMETER :: SRNAME = 'LA_GESV'
!     .. Local Scalars ..
      INTEGER :: LD, LINFO, NRHS, N
!     .. Local Pointers ..
      INTEGER, POINTER :: LPIV(:)
!     .. Intrinsic Functions ..
!     INTRINSIC ALLOCATE, DEALLOCATE, MAX, PRESENT, SIZE
      INTRINSIC MAX, PRESENT, SIZE
!
!     .. Executable Statements ..
!
!     Test the arguments
!
```

```
      LINFO = 0
      N = SIZE(A, 1)
      IF( SIZE( A, 2 ) /= N )THEN
         LINFO = -1
      ELSE IF( SIZE( B, 1 ) /= N )THEN
         LINFO = -2
      ELSE
         IF( PRESENT(IPIV) )THEN
            IF( SIZE(IPIV) /= N ) LINFO = -3
         END IF
      END IF
!
      IF( LINFO == 0 )THEN
         LD = MAX( 1, N )
         NRHS = SIZE(B,2)
         IF( PRESENT(IPIV) )THEN
            LPIV => IPIV
         ELSE
            ALLOCATE(LPIV(N))
         END IF
!
!        Call LAPACK77 routine
!
         CALL GESV_F77( N, NRHS, A, LD, LPIV, B, LD, LINFO )
!
         IF( .NOT.PRESENT(IPIV) ) DEALLOCATE(LPIV)
      END IF
!
      CALL ERINFO(LINFO,SRNAME,INFO)
!
   END SUBROUTINE SGESV_F90
```