PSBLAS-2.0 User's guide

 $A\ reference\ guide\ for\ the\ Parallel\ Sparse\ BLAS\\ library$

by Salvatore Filippone and Alfredo Buttari

"Tor Vergata" University of Rome. March 10, 2006

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1 Introduction

The PSBLAS library, developed with the aim to facilitate the parallelization of computationally intensive scientific applications, is designed to address parallel implementation of iterative solvers for sparse linear systems through the distributed memory paradigm. It includes routines for multiplying sparse matrices by dense matrices, solving block diagonal systems with triangular diagonal entries, preprocessing sparse matrices, and contains additional routines for dense matrix operations. The current implementation of PSBLAS addresses a distributed memory execution model operating with message passing. However, the overall design does not preclude different implementation paradigms, such as those based on a shared memory model.

The PSBLAS library is internally implemented in a mixture of Fortran 77 and Fortran 95 [?] programming languages. A similar approach has been advocated by a number of authors, e.g. [?]. Moreover, the Fortran 95 facilities for dynamic memory management and interface overloading greatly enhance the usability of the PSBLAS subroutines. In this way, the library can take care of runtime memory requirements that are quite difficult or even impossible to predict at implementation or compilation time. The following presentation of the PSBLAS library follows the general structure of the proposal for serial Sparse BLAS [?], which in its turn is based on the proposal for BLAS on dense matrices [?, ?, ?].

The applicability of sparse iterative solvers to many different areas causes some terminology problems because the same concept may be denoted through different names depending on the application area. The PSBLAS features presented in this section will be discussed mainly in terms of finite difference discretizations of Partial Differential Equations (PDEs). However, the scope of the library is wider than that: for example, it can be applied to finite element discretizations of PDEs, and even to different classes of problems such as nonlinear optimization, for example in optimal control problems.

The design of a solver for sparse linear systems is driven by many conflicting objectives, such as limiting occupation of storage resources, exploiting regularities in the input data, exploiting hardware characteristics of the parallel platform. To achieve an optimal communication to computation ratio on distributed memory machines it is essential to keep the *data locality* as high as possible; this can be done through an appropriate data allocation strategy. The choice of the preconditioner is another very important factor that affects efficiency of the implemented application. Optimal data distribution requirements for a given preconditioner may conflict with distribution requirements of the rest of the solver. Finding the optimal trade-off may be very difficult because it is application dependent. Possible solution to these

problems and other important inputs to the development of the PSBLAS software package has come from an established experience in applying the PSBLAS solvers to computational fluid dynamics applications.

2 General overview

The PSBLAS library is designed to handle the implementation of iterative solvers for sparse linear systems on distributed memory parallel computers. The system coefficient matrix A must be square; it may be real or complex, nonsymmetric, and its sparsity pattern needs not to be symmetric. The serial computation parts are based on the serial sparse BLAS, so that any extension made to the data structures of the serial kernels is available to the parallel version. The overall design and parallelization strategy have been influenced by the structure of the ScaLAPACK parallel library [?]. The layered structure of the PSBLAS library is shown in figure 1; lower layers of the library indicate an encapsulation relationship with upper layers. The ongoing discussion focuses on the Fortran 95 layer immediately below the application layer; two examples of iterative solvers built through the PSBLAS routines, will be also given in Section ??. The serial parts of the computation on each process are executed through calls to the serial sparse BLAS subroutines. In a similar way, the inter-process message exchanges are implemented through the Basic Linear Algebra Communication Subroutines (BLACS) library [?] that guarantees a portable and efficient communication layer. The Message Passing Interface code is encapsulated within the BLACS layer. However, in some cases, MPI routines are directly used either to improve efficiency or to implement communication patterns for which the BLACS package doesn't provide any method.

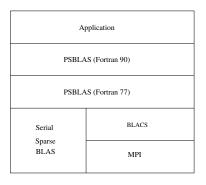


Figure 1: PSBLAS library components hierarchy.

The PSBLAS library consists of two classes of subroutines that is, the *computational routines* and the *auxiliary routines*. The computational routine set includes:

- Sparse matrix by dense matrix product;
- Sparse triangular systems solution for block diagonal matrices;
- Vector and matrix norms;
- Dense matrix sums;
- Dot products.

The auxiliary routine set includes:

- Communication descriptors allocation;
- Dense and sparse matrix allocation;
- Dense and sparse matrix build and update;
- Sparse matrix and data distribution preprocessing.

The following naming scheme has been adopted for all the symbols internally defined in the PSBLAS software package:

- all the symbols (i.e. subroutine names, data types...) are prefixed by psb_
- all the data type names are suffixed by _type
- all the constant values are suffixed by _
- all the subroutine names follow the rule psb_xxname where xx can be either:
 - ds: the routine is related to dense data,
 - sp: the routine is related to sparse data,
 - cd: the routine is related to communication descriptor (see 3).

For example the psb_dsins, psb_spins and psb_cdins perform the same action (see ??) on dense matrices, sparse matrices and communication descriptors respectively. Interface overloading allows the usage of the same subroutine interfaces for both real and complex data.

3 Data Structures

In this chapter are illustrated data structures used for definition of routines interfaces. This include data structure for sparse matrix, communication descriptor and preconditioner. These data structures are used for calling PSBLAS routines in Fortran 90 language and will be used to next chapters containing these callings. Their definitions are included in the modules psb_spmat_type, psb_descriptor_type and psb_prec_type.

3.1 Sparse Matrix data structure

The psb_spmat_type data structure contains all information about local portion of the sparse matrix and its storage mode. Many of this fields are set in fully-transparent mode by PSBLAS-TOOLS routines when inserting a new sparse matrix, user must set only fields which describe matrix storage mode (see § ??).

Fields contained in Sparse matrix structures are:

- ${f aspk}$ Contains values of the local distributed sparse matrix.
 - Specified as: a pointer to an array of rank one of type corresponding to matrix entries type .
- ia1 Holds integer information on distributed sparse matrix. Actual information will depend on data format used.
 - Specified as: a pointer to an integer array of rank one.
- ia2 Holds integer information on distributed sparse matrix. Actual information will depend on data format used.
 - Specified as: a pointer to an integer array of rank one.
- infoa On entry can hold auxiliary information on distributed sparse matrix. Actual information will depend on data format used.
 - Specified as: integer array of length 10.
- **fida** Defines the format of the distributed sparse matrix.
 - Specified as: a string of length 5
- **descra** Describe the characteristic of the distributed sparse matrix.
 - Specified as: array of character of length 9.
- **pl** Specifies the local row permutation of distributed sparse matrix. If pl(1) is equal to 0, then there isn't row permutation.
 - Specified as: pointer to integer array of dimension equal to number of local row (matrix_data[psb_n_row_])

- pr Specifies the local column permutation of distributed sparse matrix. If PR(1) is equal to 0, then there isn't column permutation. Specified as: pointer to integer array of dimension equal to number of local row (matrix_data[psb_n_col_])
- m Number of rows; if row indices are stored explicitly, as in Coordinate Storage, should be greater than or equal to the maximum row index actually present in the sparse matrix. Specified as: integer variable.
- **k** Number of columns; if column indices are stored explicitly, as in Coordinate Storage or Compressed Sparse Rows, should be greater than or equal to the maximum column index actually present in the sparse matrix. Specified as: integer variable.

Values assumed by this fields are compatible with ref. 1 (see § ??). FORTRAN95 interface for distributed sparse matrices containing double precision real entries is defined as in figure 2.

Figure 2: The PSBLAS defined data type that contains a sparse matrix.

The following two cases are among the most commonly used:

fida="CSR" Compressed storage by rows. In this case the following should hold:

- 1. ia2(i) contains the index of the first element of row i; the last element of the sparse matrix is thus stored at index ia2(m+1) 1. It should contain m+1 entries in nondecreasing order (strictly increasing, if there are no empty rows).
- 2. ia1(j) contains the column index and aspk(j) contains the corresponding coefficient value, for all $ia2(1) \le j \le ia2(m+1) 1$.

fida="COO" Coordinate storage. In this case the following should hold:

- 1. infoa(1) contains the number of nonzero elements in the matrix;
- 2. For all $1 \le j \le infoa(1)$, the coefficient, row index and column index are stored into apsk(j), ia1(j) and ia2(j) respectively.

3.2 Descriptor data structure

All the general matrix informations and elements to be exchanged among processes are stored within a data structure of the type psb_desc_type. Every structure of this type is associated to a sparse matrix, it contains data about general matrix informations and elements to be exchanged among processes.

It is not necessary for the user to know the internal structure of psb_desc_type, it is set in fully-transparent mode by PSBLAS-TOOLS routines when inserting a new sparse matrix, however the definition of the descriptor is the following.

matrix_data includes general information about matrix and BLACS grid.

More precisely:

matrix_data[psb_dec_type_] Identifies the decomposition type (global); the actual values are internally defined, so they should never be accessed directly.

matrix_data[psb_ctxt_] Communication context as returned by the BLACS (global).

matrix_data[psb_m_] Total number of equations (global).

matrix_data[psb_n_] Total number of variables (global).

matrix_data[psb_n_row_] Number of grid variables owned by the current process (local); equivalent to the number of local rows in the sparse coefficient matrix.

matrix_data[psb_n_col_] Total number of grid variables read by the current process (local); equivalent to the number of local columns in the sparse coefficient matrix. They include the halo.

Specified as: a pointer to integer array of dimension 10.

halo_index A list of the halo and boundary elements for the current process to be exchanged with other processes; for each processes with which it is necessary to communicate:

- 1. Process identifier;
- 2. Number of points to be received;
- 3. Indices of points to be received;
- 4. Number of points to be sent;
- 5. Indices of points to be sent;

The list may contain an arbitrary number of groups; its end is marked by a -1.

Specified as: a pointer to an integer array of rank one.

ovrlap_index A list of the overlap elements for the current process, organized in groups like the previous vector:

- 1. Process identifier;
- 2. Number of points to be received;
- 3. Indices of points to be received;
- 4. Number of points to be sent;
- 5. Indices of points to be sent;

The list may contain an arbitrary number of groups; its end is marked by a -1.

Specified as: a pointer to an integer array of rank one.

ovrlap_index For all overlap points belonging to the current process:

- 1. Overlap point index;
- 2. Number of processes sharing that overlap points;

The list may contain an arbitrary number of groups; its end is marked by a -1.

Specified as: a pointer to an integer array of rank one.

 loc_to_glob each element i of this array contains global identifier of the local variable i.

Specified as: a pointer to an integer array of rank one.

glob_to_loc if global variable i is read by current process then element i contains local index correspondent to global variable i; else element i contains -1 (NULL) value.

Specified as: a pointer to an integer array of rank one.

FORTRAN95 interface for psb_desc_type structures is therefore defined as follows:

```
type psb_desc_type
  integer, pointer :: matrix_data(:), halo_index(:)
  integer, pointer :: overlap_elem(:), overlap_index(:)
  integer, pointer :: loc_to_glob(:), glob_to_loc(:)
end type psb_desc_type
```

Figure 3: The PSBLAS defined data type that contains the communication descriptor.

3.3 Preconditioner data structure

PSBLAS-2.0 offers the possibility to use many different types of preconditioning schemes. Besides the simple well known preconditioners like Diagonal Scaling or Block Jacobi (with ILU(0) incomplete factorization) also more complex preconditioning methods are implemented like the Additive Schwarz and Two-Level ones. A preconditioner is held in the psb_prec_type data structure which depends on the psb_base_prec reported in figure 4. The psb_base_prec data type may contain a simple preconditioning matrix with the associated communication descriptor which may be different than the system communication descriptor in the case of parallel preconditioners like the Additive Schwarz one. Then the psb_prec_type may contain more than one preconditioning matrix like in the case of Two-Level (in general Multi-Level) preconditioners. The user can choose the type of preconditioner to be used by means of the psb_precset subroutine; once the type of preconditioning method is specified, along with all the parameters that characterize it, the preconditioner data structure can be built using the psb_precbuild subroutine. This data structure wants to be flexible enough to easily allow the implementation of new kind of preconditioners. The values contained in the iproparm and dproparm define tha type of preconditioner along with all the parameters related to it; thus, iprcparm and dprcparm define how the other records have to be interpreted.

```
type psb_base_prec
  type(psb_spmat_type), pointer :: av(:) => null()
  real(kind(1.d0)), pointer :: d(:) \Rightarrow null()
  type(psb_desc_type), pointer :: desc_data => null()
                               :: iprcparm(:) => null()
  integer, pointer
  real(kind(1.d0)), pointer :: dprcparm(:) => null()
  integer, pointer
                                :: perm(:) => null()
  integer, pointer
                                :: mlia(:) => null()
                               :: invperm(:) => null()
  integer, pointer
                         :: nlaggr(:) => null()
  integer, pointer
  type(psb_spmat_type), pointer :: aorig => null()
  real(kind(1.d0)), pointer
                                :: dorig(:) => null()
end type psb_base_prec
type psb_prec_type
  type(psb_base_prec), pointer :: baseprecv(:) => null()
                               :: prec, base_prec
   integer
end type psb_prec_type
```

Figure 4: The PSBLAS defined data type that contains a preconditioner.

4 Algebraic routines

psb_geaxpby—General Dense Matrix Sum

This subroutine is an interface to the computational kernel for dense matrix sum:

$$y \leftarrow \alpha \ x + \beta y$$

where:

x represents the global dense submatrix $x_{:,jx:jx+n-1}$

y represents the global dense submatrix $y_{:,jy:jy+n-1}$

Syntax

call psb_geaxpby (alpha, x, beta, y, $desc_a$, info)

call psb_geaxpby (alpha, x, beta, y, desc_a, info, n, jx, jy)

x, y, α, β	Subroutine
Single Precision Real	psb_geaxpby
Long Precision Real	$psb_geaxpby$
Long Precision Complex	$psb_geaxpby$

Table 1: Data types

On Entry

alpha the scalar α .

Scope: **global**Type: **required**

Specified as: a number of the data type indicated in Table 1.

 \mathbf{x} the local portion of global dense matrix x.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 1. The rank of x must be the same of y.

beta the scalar β .

Scope: **global** Type: **required**

Specified as: a number of the data type indicated in Table 1.

 \mathbf{y} the local portion of the global dense matrix y.

Scope: **local** Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of the type indicated in Table 1. The rank of y be the same of x.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

n number of columns in dense submatrices x and y.

Scope: **global**

Type: **optional**; can only be present if x and y are of rank 2.

Default: min(size(x,2), size(y,2)). Specified as: an integer variable n > 0.

 $\mathbf{j}\mathbf{x}$ the column index of the global dense matrix x, identifying the first column of the submatrix x.

Scope: global

Type: **optional**; can only be present if x and y are of rank 2.

Default: jx = 1.

Specified as: an integer variable $jx \geq 1$.

jy the column index of the global dense matrix y, identifying the first column of the submatrix y.

Scope: global

Type: **optional**; can only be present if x and y are of rank 2.

Default: jy = 1.

Specified as: an integer variable $jy \ge 1$.

On Return

 \mathbf{y} the local portion of result submatrix y.

Scope: **local**Type: **required**

Specified as: a rank one or two array containing numbers of the type indicated in Table 1.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

$psb_gedot—Dot Product$

This function computes dot product between two vectors x and y. If x and y are double precision real or single precision real vectors computes dot-product as:

$$dot \leftarrow x^T y$$

Else if x and y are double precision complex vectors then computes dot-product as:

$$dot \leftarrow x^H y$$

where:

x represents the global subvector $x_{:,jx}$

y represents the global subvector $y_{:,jy}$

Syntax

 $psb_gedot(x, y, desc_a, info)$

 $psb_gedot(x, y, desc_a, info, jx, jy)$

dot, x, y	Function
Single Precision Real	psb_gedot
Long Precision Real	psb_gedot
Long Precision Complex	psb_gedot

Table 2: Data types

On Entry

 ${f x}$ the local portion of global dense matrix x. This function computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a pointer to array of rank one or two containing numbers of type specified in Table 2. The rank of x must be the same of y.

y the local portion of global dense matrix y. This function computes the location of the first element of local subarray used, based on iy, jy and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a pointer to array of rank one or two containing numbers of type specified in Table 2. The rank of y must be the same of x.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

jx the column index of global dense matrix x, identifying the column of subvector x.

Scope: global

Type: **optional**; can only be present if x and y are of rank 2.

Default: jx = 1.

jy the column index of global dense matrix y, identifying the column of subvector y.

Scope: global

Type: **optional**; can only be present if x and y are of rank 2.

Default: jy = 1.

Specified as: an integer variable $jy \ge 1$.

On Return

Function value is the dot product of subvectors x and y.

Scope: global

Specified as: a number of the data type indicated in Table 2.

info the local portion of result submatrix y.

Scope: **local**Type: **required**

psb_gedot—Generalized Dot Product

This subroutine computes a series of dot products among the columns of two dense matrices x and y:

$$res(i) \leftarrow x(:,i)^T y(:,i)$$

If the matrices are complex, then the usual convention applies, i.e. the conjugate transpose of x is used. If x and y are of rank one, then res is a scalar, else it is a rank one array.

Syntax

 $psb_gedot (res, x, y, desc_a, info)$

res, x, y	Subroutine
Single Precision Real	$\operatorname{psb_gedot}$
Long Precision Real	psb_gedot
Long Precision Complex	psb_gedot

Table 3: Data types

On Entry

 \mathbf{x} the local portion of global dense matrix x.

Scope: **local** Type: **required**

Specified as: a pointer to array of rank one or two containing numbers of type specified in Table 3. The rank of x must be the same of y.

 \mathbf{y} the local portion of global dense matrix y.

Scope: **local** Type: **required**

Specified as: a pointer to array of rank one or two containing numbers of type specified in Table 3. The rank of y must be the same of x.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

On Return

res is the dot product of subvectors x and y.

 $Scope: \ \mathbf{global}$

Specified as: a number or a rank-one array of the data type indicated

in Table 2.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_geamax—Infinity-Norm of Vector

This function computes the infinity-norm of a vector x.

If x is double precision real or single precision real vector computes infinity norm as:

$$amax \leftarrow \max_{i} |x_i|$$

else if x is double precision complex vector then computes infinity-norm as:

$$amax \leftarrow \max_{i} (|re(x_i)| + |im(x_i)|)$$

where:

x represents the global subvector $x_{:,jx}$

Syntax

$$psb_geamax (x, desc_a, info)$$

$$psb_geamax (x, desc_a, info, jx)$$

amax	x	Function
Single Precision Real	Single Precision Real	psb_geamax
Long Precision Real	Long Precision Real	psb_geamax
Long Precision Real	Long Precision Complex	psb_geamax

Table 4: Data types

On Entry

 \mathbf{x} the local portion of global dense matrix x. This function computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 4.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

 $\mathbf{j}\mathbf{x}$ the column index of global dense matrix x, identifying the column of

subvector x. Scope: **global**

Type: **optional**; can only be present if x is of rank 2.

Default: jx = 1

Specified as: an integer variable $jx \ge 1$.

On Return

Function value is the infinity norm of subvector x.

Scope: global

Specified as: a number of the data type indicated in Table 4.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_geamax—Generalized Infinity Norm

This subroutine computes a series of infinity norms on the columns of a dense matrix x:

$$res(i) \leftarrow \max_{k} |x(k,i)|$$

Syntax

 $psb_geamax (res, x, desc_a, info)$

res	x	Subroutine
Single Precision Real	Single Precision Real	psb_geamax
Long Precision Real	Long Precision Real	psb_geamax
Long Precision Real	Long Precision Complex	psb_geamax

Table 5: Data types

On Entry

 \mathbf{x} the local portion of global dense matrix x.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 5.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

On Return

res is the infinity norm of the columns of x.

Scope: global

Specified as: a number or a rank-one array of the data type indicated in Table 4.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_geasum —1-Norm of Vector

This function computes the 1-norm of a vector x.

If x is double precision real or single precision real vector computes 1-norm as:

$$asum \leftarrow ||x_i||$$

else if x ic double precision complex vector then computes 1-norm as:

$$asum \leftarrow ||re(x)||_1 + ||im(x)||_1$$

where:

x represents the global subvector $x_{:,jx}$

Syntax

 $psb_geasum (x, desc_a, info)$

 $psb_geasum (x, desc_a, info, jx)$

dot, x, y	Function
Single Precision Real	psb_geasum
Long Precision Real	psb_geasum
Long Precision Complex	psb_geasum

Table 6: Data types

On Entry

 ${f x}$ the local portion of global dense matrix x. This function computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 6.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

 $\mathbf{j}\mathbf{x}$ the column index of global dense matrix x, identifying the column of

subvector x. Scope: **global**

Type: **optional**; can only be present if x is of rank 2.

Default: jx = 1

Specified as: an integer variable $jx \ge 1$.

On Return

Function value is the 1-norm of subvector x.

Scope: **global**

Specified as: a number of the data type indicated in Table 6.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_genrm2—2-Norm of Vector

This function computes the 2-norm of a vector x.

If x is double precision real or single precision real vector computes 2-norm as:

$$nrm2 \leftarrow \sqrt{x^Tx}$$

else if x is double precision complex vector then computes 2-norm as:

$$nrm2 \leftarrow \sqrt{x^H x}$$

where:

x represents the global subvector $x_{:,jx}$

nrm2, x	Function
Single Precision Real	psb_genrm2
Long Precision Real	psb_genrm2
Long Precision Complex	psb_genrm2

Table 7: Data types

Syntax

 psb_genrm2 ($x, desc_a, info$)

 psb_genrm2 ($x, desc_a, info, jx$)

On Entry

 ${f x}$ the local portion of global dense matrix x. This function computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 7.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

 $\mathbf{j}\mathbf{x}$ the column index of global dense matrix x, identifying the column of

subvector x. Scope: **global**

Type: **optional**; can only be present if x is of rank 2.

Default: jx = 1

Specified as: an integer variable $jx \ge 1$.

On Return

Function Value is the 2-norm of subvector x.

Scope: **global**Type: **required**

Specified as: a number of the data type indicated in Table 7.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_spnrmi—Infinity Norm of Sparse Matrix

This function computes the infinity-norm of a matrix A:

$$nrmi \leftarrow ||A||_{\infty}$$

where:

A represents the global matrix A

nrmi, A	Function
Single Precision Real	psb_spnrmi
Long Precision Real	psb_spnrmi
Long Precision Complex	psb_spnrmi

Table 8: Data types

Syntax

psb_spnrmi $(A, desc_a, info)$

On Entry

 \mathbf{a} the local portion of the global sparse matrix A.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_spmat_type.

 $\mathbf{desc_a}$ contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

On Return

Function value is the infinity-norm of sparse submatrix A.

Scope: global

Specified as: a number of the data type indicated in Table 8.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

psb_spmm—Sparse Matrix by Dense Matrix Product

This subroutine computes the Sparse Matrix by Dense Matrix Product:

$$y \leftarrow \alpha P_r A P_c x + \beta y \tag{1}$$

$$y \leftarrow \alpha P_r A^T P_c x + \beta y \tag{2}$$

$$y \leftarrow \alpha P_r A^H P_c x + \beta y \tag{3}$$

where:

x is the global dense submatrix $x_{:,jx:jx+k-1}$

y is the global dense submatrix $y_{:,jy:jy+k-1}$

A is the global sparse submatrix A

 P_r, P_c are the permutation matrices.

A, x, y, α, β	Subroutine
Single Precision Real	psb_spmm
Long Precision Real	psb_spmm
Long Precision Complex	psb_spmm

Table 9: Data types

Syntax

CALL psb_spmm (alpha, a, x, beta, y, desc_a, info)

CALL psb_spmm (alpha, a, x, beta, y,desc_a, info, trans, k, jx, jy, work)

On Entry

alpha the scalar α .

Scope: **global**Type: **required**

Specified as: a number of the data type indicated in Table 9.

 \mathbf{a} the local portion of the sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

 \mathbf{x} the local portion of global dense matrix x. This subroutine computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 9. The rank of x must be the same of y.

beta the scalar β .

Scope: **global**Type: **required**

Specified as: a number of the data type indicated in Table 9.

y the local portion of global dense matrix y. This subroutine computes the location of the first element of local subarray used, based on jy and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 9. The rank of y must be the same of x.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

trans indicate what kind of operation to perform.

trans = N the operation is specified by equation 1

trans = T the operation is specified by equation 2

trans = C the operation is specified by equation 3

Scope: **global** Type: **optional** Default: trans = N

Specified as: a character variable.

 \mathbf{k} number of columns in dense submatrices x and y.

Scope: **global** Type: **optional**

Default: min(size(x,2)-jx+1,size(y,2)-jy+1)

Specified as: an integer variable $k \geq 1$.

 $\mathbf{j}\mathbf{x}$ the column index of global dense matrix x, identifying the column of subvector x.

Scope: global

Type: **optional**; can only be present if x is of rank 2.

Default: iy = 1

Specified as: an integer variable $jx \geq 1$.

jy the column index of global dense matrix y, identifying the column of

subvector y. Scope: **global**

Type: **optional**; can only be present if y is of rank 2.

Default: jy = 1

Specified as: an integer variable $jy \ge 1$.

work the work array.

Scope: local

Specified as: a rank one array of the same type of x and y with the

POINTER attribute.

On Return

 \mathbf{y} the local portion of result submatrix y.

Scope: **local**Type: **required**

Specified as: a pointer to array of rank one or two containing numbers

of type specified in Table 9.

info the local portion of result submatrix y.

Scope: **local**Type: **required**

psb_spsm—Triangular System Solve

This subroutine computes the Triangular System Solve:

$$y \leftarrow \alpha P_r T^{-1} P_c x + \beta y$$

$$y \leftarrow \alpha D P_r T^{-1} P_c x + \beta y$$

$$y \leftarrow \alpha P_r T^{-1} P_c D x + \beta y$$

$$y \leftarrow \alpha P_r T^{-T} P_c x + \beta y$$

$$y \leftarrow \alpha D P_r T^{-T} P_c x + \beta y$$

$$y \leftarrow \alpha D P_r T^{-T} P_c D x + \beta y$$

$$y \leftarrow \alpha P_r T^{-H} P_c x + \beta y$$

$$y \leftarrow \alpha D P_r T^{-H} P_c x + \beta y$$

$$y \leftarrow \alpha D P_r T^{-H} P_c x + \beta y$$

$$y \leftarrow \alpha P_r T^{-H} P_c x + \beta y$$

$$y \leftarrow \alpha P_r T^{-H} P_c D x + \beta y$$

where:

x is the global dense submatrix $x_{:,jx:jx+n-1}$

y is the global dense submatrix $y_{:,jy:jy+n-1}$

T is the global sparse block triangular submatrix T

D is the scaling diagonal matrix.

 P_r, P_c are the permutation matrices.

Syntax

CALL psb_spsm (alpha, t, x, beta, y, desc_a, info)

CALL psb_spsm

(alpha, t, x, beta, y, desc_a, info, trans, unit, choice, diag, n, jx, jy, work)

On Entry

$T, x, y, D, \alpha, \beta$	Subroutine
Single Precision Real	psb_spsm
Long Precision Real	psb_spsm
Long Precision Complex	psb_spsm

Table 10: Data types

alpha the scalar α .

Scope: **global** Type: **required**

Specified as: a number of the data type indicated in Table 10.

 \mathbf{t} the global portion of the sparse matrix T.

Scope: **local**Type: **required**

Specified as: a structured data type specified in § 3.

 \mathbf{x} the local portion of global dense matrix x. This subroutine computes the location of the first element of local subarray used, based on jx and the field $matrix_data$ of $desc_a$.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 10. The rank of x must be the same of y.

beta the scalar β .

Scope: **global** Type: **required**

Specified as: a number of the data type indicated in Table 10.

y the local portion of global dense matrix y. This subroutine computes the location of the first element of local subarray used, based on jy and the field $matrix_data$ of $desc_a$.

Scope: **local** Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 10. The rank of y must be the same of x.

desc_a contains data structures for communications.

Scope: local

Type: required

Specified as: a structured data of type psb_desc_type.

trans specify with *unitd* the operation to perform.

trans = 'N' the operation is with no transposed matrix

trans = 'T' the operation is with transposed matrix.

trans = 'C' the operation is with conjugate transposed matrix.

Scope: **global** Type: **optional** Default: trans = N

Specified as: a character variable.

unitd specify with *trans* the operation to perform.

unitd = 'U' the operation is with no scaling

unitd = 'L' the operation is with left scaling

unitd = 'R' the operation is with right scaling.

Scope: **global** Type: **optional** Default: unitd = U

Specified as: a character variable.

choice specify whether a cleanup of the overlapped elements is required on exit.

choice = .false. no cleanup on exit

choice = .true. cleanup on exit.

Scope: **global**Type: **optional**

Default: choice = .true.

Specified as: a logical variable.

diag the diagonal scaling matrix.

Scope: local
Type: optional

Default: diag(1) = 1(noscaling)

Specified as: a rank one array containing numbers of the type indicated

in Table 10.

n number of columns in dense submatrices x and y.

Scope: **global** Type: **optional**

Default: min(size(x,2)-jx+1,size(y,2)-jy+1)

Specified as: an integer variable $n \geq 0$.

 $\mathbf{j}\mathbf{x}$ the column index of global dense matrix x, identifying the column of subvector x.

Scope: global

Type: **optional**; can only be present if x is of rank 2.

Default: jx = 1

Specified as: an integer variable $jx \geq 1$.

jy the column index of global dense matrix y, identifying the column of subvector y.

Scope: **global**

Type: **optional**; can only be present if y is of rank 2.

Default: jy = 1

Specified as: an integer variable $jy \ge 1$.

Scope: global

Specified as: a number of the data type indicated in Table 10.

work the work array.

Scope: **local** Type: **optional**

Specified as: a rank one array of the same type of x with the POINTER

attribute.

On Return

y the local portion of global dense matrix y. This subroutine computes the location of the first element of local subarray used, based on jy and the field $matrix_data$ of $desc_a$.

Scope: **local** Type: **required**

Specified as: a pointer to array of rank one or two containing numbers of type specified in Table 10.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

An integer value that contains an error code.

5 Communication routines

psb_halo—Halo Data Communication

These subroutines restore a consistent status for the halo elements, and (optionally) scale the result:

$$x \leftarrow \alpha x$$

where:

x is a global dense submatrix.

α, x	Subroutine
Single Precision Real	psb_halo
Long Precision Real	psb_halo
Long Precision Complex	psb_halo

Table 11: Data types

Syntax

CALL psb_halo $(x, desc_a, info)$

CALL psb_halo (x, desc_a, info, alpha, work)

On Entry

 \mathbf{x} global dense matrix x.

Scope: **local**Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 11.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

alpha the scalar α .

Scope: **global** Type: **optional** Default: alpha = 1

Specified as: a number of the data type indicated in Table 11.

work the work array.

Scope: **local**Type: **optional**

Specified as: a rank one array of the same type of x with the POINTER

attribute.

On Return

 \mathbf{x} global dense result matrix x.

Scope: **local** Type: **required**

Returned as: a rank one or two array with the POINTER attribute

containing numbers of type specified in Table 11.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

An integer value that contains an error code.

psb_ovrl—Overlap Update

These subroutines restore a consistent status for the overlap elements:

$$x \leftarrow Qx$$

where:

x is the global dense submatrix x

Q is the overlap operator; it is the composition of two operators P_a and P^T .

\overline{x}	Subroutine
Single Precision Real	$\operatorname{psb_ovrl}$
Long Precision Real	psb_ovrl
Long Precision Complex	psb_ovrl

Table 12: Data types

Syntax

CALL psb_ovrl $(x, desc_a, info)$

CALL psb_ovrl

 $(x, desc_a, info, choice=choice, update_type=update_type, work=work)$

On Entry

 \mathbf{x} global dense matrix x.

Scope: **local** Type: **required**

Specified as: a rank one or two array with the POINTER attribute containing numbers of type specified in Table 12.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

choice specify if exchange overlap elements.

choice = .true. exchange overlap elements, i.e. apply operator P^T ;

choice = .false. don't exchange overlap elements

Scope: **global**Type: **optional**

Default: choice = .true.

Specified as: a logical variable.

 $update_type = 1$ normal update P_a ;

update_type = 2 square root update $\sqrt{P_a}$;

Scope: global

Default: $update_type = .true$.

Scope: global

Specified as: a integer variable.

work the work array.

Scope: local Type: optional

Specified as: a one dimensional array of the same type of x.

On Return

 \mathbf{x} global dense result matrix x.

Scope: **local**Type: **required**

Specified as: a pointer to array of rank one or two containing numbers

of type specified in Table 12.

info the local portion of result submatrix y.

Scope: **local**Type: **required**

An integer value that contains an error code.

Usage notes

1. If there is no overlap in the data distribution, no operations are performed;

- 2. The operator P^T performs the reduction sum of overlap elements; it is the inverse of a "stretch" operator P that replicates overlap elements, accounting for the physical replication of data;
- 3. The operator P_a performs a scaling on the overlap elements by the amount of replication; thus, when combined with the reduction operator, it implements the average of replicated elements over all of their instances.
- 4. The square root update option makes it possible to apply the following operator:

 $x \leftarrow \sqrt{P_a} P^T K^{-1} P \sqrt{P_a} x$

In the case of a symmetric K, this preserves simmetry of the overall preconditioner, which would otherwise be destroyed.

psb_gather—Gather Global Dense Matrix

These subroutines collect the portions of global dense matrix distributed over all process into one single array stored on one process.

$$glob_x \leftarrow collect(loc_x_i)$$

where:

 $glob_x$ is the global submatrix $glob_x_{iy:iy+m-1,jy:jy+n-1}$

 loc_x_i is the local portion of global dense matrix on process i.

collect is the collect function.

x_i, y	Subroutine
Single Precision Real	psb_gather
Long Precision Real	psb_gather
Long Precision Complex	psb_gather

Table 13: Data types

Syntax

call psb_gather

 $(glob_x, loc_x, desc_a, info, root, iglobx, jglobx, ilocx, jlocx, k)$

Syntax

call psb_gather (glob_x, loc_x, desc_a, info, root, iglobx, ilocx)

On Entry

 loc_x the local portion of global dense matrix $glob_x$.

Scope: **local** Type: **required**

Specified as: a rank one or two array containing numbers of the type

indicated in Table 13.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

root The process that holds the global copy. If root = -1 all the processes will have a copy of the global vector.

Scope: **global** Type: **optional**

Specified as: an integer variable $0 \le ix \le np$.

iglobx Row index to define a submatrix in glob_x into which gather the local pieces.

Scope: **global**Type: **optional**

Specified as: an integer variable $1 \le ix \le matrix_data(psb_m_)$.

jglobx Column index to define a submatrix in glob_x into which gather the local pieces.

Scope: **global** Type: **optional**

Specified as: an integer variable.

ilocx Row index to define a submatrix in loc_x that has to be gathered into glob_x.

Scope: **local**Type: **optional**

Specified as: an integer variable.

jlocx Columns index to define a submatrix in loc_x that has to be gathered into glob_x.

Scope: **global** Type: **optional**

Specified as: an integer variable.

k The number of columns to gather.

Scope: **global** Type: **optional**

Specified as: an integer variable.

On Return

glob_x The array where the local parts must be gathered.

Scope: global

Type: required

Specified as: a rank one or two array.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

An integer value that contains an error code.

psb_scatter—Scatter Global Dense Matrix

These subroutines scatters the portions of global dense matrix owned by a process to all the processes in the processes grid.

$$loc_{-}x_{i} \leftarrow scatter(glob_{-}x_{i})$$

where:

 $glob_x$ is the global submatrix $glob_x_{iy:iy+m-1,jy:jy+n-1}$

 $loc_{-}x_{i}$ is the local portion of global dense matrix on process i.

scatter is the scatter function.

x_i, y	Subroutine
Single Precision Real	psb_scatter
Long Precision Real	$psb_scatter$
Long Precision Complex	$psb_scatter$

Table 14: Data types

Syntax

call psb_scatter

(glob_x, loc_x, desc_a, info, root, iglobx, jglobx, ilocx, jlocx, k)

Syntax

call psb_scatter (glob_x, loc_x, desc_a, info, root, iglobx, ilocx)

On Entry

glob_x The array that must be scattered into local pieces.

Scope: **global** Type: **required**

Specified as: a rank one or two array.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

root The process that holds the global copy. If root = -1 all the processes

have a copy of the global vector.

Scope: **global** Type: **optional**

Specified as: an integer variable $0 \le ix \le np$.

iglobx Row index to define a submatrix in glob_x that has to be scattered

into local pieces. Scope: **global** Type: **optional**

Specified as: an integer variable $1 \le ix \le matrix_data(psb_m_)$.

jglobx Column index to define a submatrix in glob_x that has to be scattered

into local pieces.

Scope: **global**Type: **optional**

Specified as: an integer variable.

ilocx Row index to define a submatrix in loc_x into which scatter the local

piece of glob_x.
Scope: **local**

Type: optional

Specified as: an integer variable.

jlocx Columns index to define a submatrix in loc_x into which scatter the

local piece of glob_x.

Scope: **global** Type: **optional**

Specified as: an integer variable.

k The number of columns to scatter.

Scope: **global** Type: **optional**

Specified as: an integer variable.

On Return

 loc_x the local portion of global dense matrix $glob_x$.

Scope: local

Type: required

Specified as: a rank one or two array containing numbers of the type indicated in Table 14.

info the local portion of result submatrix y.

Scope: **local** Type: **required**

An integer value that contains an error code.

6 Data management and initialization routines

psb_geall—Allocates a dense matrix

Syntax

call psb_geall $(m, n, x, desc_a, info, js)$

On Entry

m The number of rows of the dense matrix to be allocated.

Scope: **local**Type: **required**

Specified as: Integer scalar.

n The number of columns of the dense matrix to be allocated.

Scope: **local**Type: **required**

Specified as: Integer scalar.

desc_a The communication descriptor.

Scope: **local** Type: **required**

Specified as: a variable of type psb_desc_type.

js The starting column.

Scope: **local**Type: **optional**

Specified as: Integer scalar.

On Return

x The dense matrix to be allocated.

Scope: **local** Type: **required**

Specified as: a one or two dimensional array.

info Error code. Scope: local

Type: required

psb_geasb—Assembly a dense matrix

Syntax

call psb_geasb $(x, desc_a, info)$

On Entry

 $\mathbf{desc}_{-}\mathbf{a}$ The communication descriptor.

Scope: **local**Type: **required**

Specified as: a variable of type psb_desc_type.

On Return

 \mathbf{x} The dense matrix to be assembled.

Scope: **local** Type: **required**

Specified as: a one or two dimensional array.

info Error code.

Scope: **local** Type: **required**

psb_csrp—Applies a right permutation to a sparse matrix

Syntax

call psb_csrp (trans, iperm, a, desc_a, info)

On Entry

trans A character that specifies whether to permute A or A^T .

Scope: **local**Type: **required**

Specified as: a single character with value 'N' for A or 'T' for A^T .

iperm An integer array containing permutation information.

Scope: **local**Type: **required**

Specified as: an integer one-dimensional array.

a The sparse matrix to be permuted.

Scope: **local**Type: **required**

Specified as: a psb_spmat_typevariable.

 $desc_a$ The communication descriptor of type psb_desc_type .

Scope: **local**Type: **required**

Specified as: a variable of type psb_desc_type.

On Return

info Error code.

Scope: **local** Type: **required**

psb_cdprt—Prints a descriptor

Syntax

call psb_cdprt (iout, desc_a, glob, short)

On Entry

iout An integer that defines the output unit. Scope: local

Type: required

Specified as: Integer scalar.

desc_a The communication descriptor of type psb_desc_typethat must be

printed.

Scope: **local**

 ${\bf Type:\ required}$

Specified as: a variable of type psb_desc_type.

On Return

glob ??????

short ??????

psb_gefree—Frees a dense matrix

Syntax

call psb_gefree ($x, desc_a, info$)

On Entry

 ${f x}$ The dense matrix to be freed.

Scope: **local** Type: **required**

Specified as: a one or two dimensional array.

 $\mathbf{desc}_{-\mathbf{a}}$ The communication descriptor.

Scope: **local**Type: **required**

Specified as: a variable of type psb_desc_type.

On Return

info Error code.

Scope: **local**Type: **required**

psb_gelp—Applies a left permutation to a dense matrix

Syntax

call psb_gelp (trans, iperm, x, desc_a, info)

On Entry

trans A character that specifies whether to permute A or A^T .

Scope: **local**Type: **required**

Specified as: a single character with value 'N' for A or 'T' for A^T .

iperm An integer array containing permutation information.

Scope: **local**Type: **required**

Specified as: an integer one-dimensional array.

 \mathbf{x} The dense matrix to be permuted.

Scope: **local**Type: **required**

Specified as: a one or two dimensional array.

 $\mathbf{desc}_{-\mathbf{a}}$ The communication descriptor.

Scope: **local**Type: **required**

Specified as: a variable of type psb_desc_type.

On Return

info Error code.

Scope: **local** Type: **required**

psb_spins—Insert a cloud of elements into a sparse matrix

Syntax

call psb_spins (nz, ia, ja, val, a, desc_a, info, is, js)

On Entry

nz the number of elements to be inserted.

Scope:local.

Type:required.

Specified as: an integer scalar.

ia the row indices of the elements to be inserted.

Scope:local.

Type:required.

Specified as: an integer array of size nz.

ja the column indices of the elements to be inserted.

Scope:local.

Type:required.

Specified as: an integer array of size nz.

val the elements to be inserted.

Scope:local.

Type:required.

Specified as: an array of size nz.

 $\mathbf{desc}_{-}\mathbf{a}$ The communication descriptor.

Scope: local.

Type: required.

Specified as: a variable of type psb_desc_type.

is the starting row on matrix a.

Scope:local.

Type:optional.

js the starting column on matrix a.

Scope:local.
Type:optional

Specified as: an integer value

On Return

a the matrix into which elements will be inserted.

Scope:**local** Type:**required**

Specified as: a structured data of type psb_spmat_type.

info Error code.

Scope: **local** Type: **required**

psb_cdall—Allocates a communication descriptor

Syntax

```
call psb_cdall (m, n, parts, icontxt, desc_a, info)
call psb_cdall (m, v, icontxt, desc_a, info, flag)
```

On Entry

m the number of rows of the problem.

Scope:global.

 ${\bf Type:} {\bf required}.$

Specified as: an integer value.

 ${f n}$ the number of columns of the problem.

Scope:global.

Type:required.

Specified as: an integer value.

parts the subroutine that defines the partitioning scheme.

Scope:global.

Type:required.

Specified as: a subroutine as described in ???

icontxt the communication context.

Scope:global.

Type:required.

Specified as: an integer value.

On Return

desc_a the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

 $\mathbf{info} \ \mathrm{Error} \ \mathrm{code}. \ \mathrm{Scope:} \ \mathbf{local}$

Type: required

${\bf psb_cdasb--Communication\ descriptor} \\ {\bf assembly\ routine}$

Syntax

call psb_cdasb ($desc_a$, info)

On Entry

 $\mathbf{desc}_{-}\mathbf{a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

info Error code. Scope: local

Type: required

Specified as: an integer variable.

 arg

$psb_cdcpy\\--Copies\ a\ communication\\ descriptor$

Syntax

call psb_cdcpy (desc_out, desc_a, info)

On Entry

 $\mathbf{desc}_{-\mathbf{a}}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

desc_out the communication descriptor copy.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

info Error code. Scope: local

Type: required

$\begin{array}{l} psb_cdfree \\ \hline -Frees\ a\ communication \\ descriptor \end{array}$

Syntax

call psb_cdfree ($desc_a$, info)

On Entry

 $\mathbf{desc}_{-\mathbf{a}}$ the communication descriptor to be freed.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

info Error code. Scope: local

Type: required

psb_cdins—Comunnication descriptor insert routine

Syntax

call psb_cdins (nz, ia, ja, desc_a, info, is, js)

On Entry

nz the number of points being inserted.

Scope: **local**.

Type: **required**.

Specified as: an integer value.

ia the row indices of the points being inserted.

Scope: **local**. Type: **required**.

Specified as: an integer array of length nz.

ja the column indices of the points being inserted.

Scope: **local**. Type: **required**.

Specified as: an integer array of length nz.

is the row offset.

Scope:local.

Type:optional.

Specified as: an integer value.

js the column offset.

Scope: **local**.

Type: optional.

Specified as: an integer value.

On Return

desc_a the communication descriptor to be freed.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

 ${f info}$ Error code. Scope: ${f local}$

Type: required

psb_cdren—Applies a renumeration to a communication descriptor

Syntax

call psb_cdren (trans, iperm, desc_a, info)

On Entry

trans A character that specifies whether to permute A or A^{T} .

Scope: **local**Type: **required**

Specified as: a single character with value 'N' for A or 'T' for A^T .

iperm An integer array containing permutation information.

Scope: **local** Type: **required**

Specified as: an integer one-dimensional array.

 $\mathbf{desc}_{-\mathbf{a}}$ the communication descriptor.

Scope:**local**.
Type:**required**.

Specified as: a structured data of type psb_desc_type.

On Return

info Error code. Scope: local

Type: required

psb_spall—Allocates a sparse matrix

Syntax

call psb_spall (a, $desc_a$, info, nnz)

On Entry

 $\mathbf{desc_a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

nnz the number of nonzeroes in the matrix.

Scope: **global**. Type: **optional**.

Specified as: an integer value.

On Return

a the matrix to be allocated.

Scope:local

Type:required

Specified as: a structured data of type psb_spmat_type.

info Error code. Scope: local

Type: required

psb_spasb—Sparse matrix assembly routine

Syntax

```
call psb_spasb (a, desc_a, info, afmt, up, dup)
```

On Entry

 $\mathbf{desc}_{-}\mathbf{a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

 $\mathbf{afmt} \;\; \mathbf{the} \; \mathbf{storage} \; \mathbf{format} \; \mathbf{for} \; \mathbf{the} \; \mathbf{sparse} \; \mathbf{matrix}.$

Scope: global.

Type: optional.

Specified as: an array of characters. If not specified 'CSR' will be

assumed.

up ???.

Scope: global.

Type: optional.

Specified as: .

dup ???.

Scope: global.

Type: optional.

Specified as:

On Return

a the matrix to be assembled.

Scope:local

Type:required

Specified as: a structured data of type psb_spmat_type.

info Error code. Scope: local

Type: required

psb_spcnv—Converts a sparse matrix storage format

Syntax

call psb_spcnv (a, b, desc_a, info)

On Entry

a the matrix to be converted.

Scope:local

Type:required

Specified as: a structured data of type psb_spmat_type.

 $\mathbf{desc_a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

b the converted matrix.

Scope:local

Type:required

Specified as: a structured data of type psb_spmat_type.

info Error code. Scope: local

Type: required

psb_spfree —Frees a sparse matrix

Syntax

call psb_spfree (a, $desc_a$, info)

On Entry

a the matrix to be freed.

Scope: local

Type:required

Specified as: a structured data of type psb_spmat_type.

 $\mathbf{desc}_{-}\mathbf{a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

info Error code. Scope: local

Type: required

psb_geins—Dense matrix insertion routine

Syntax

call psb_geins (m, n, x, ix, jx, blck, desc_a, info, iblck, jblck)

On Entry

m rows number of submatrix belonging to blck to be inserted..

Scope:local.

Type:required.

Specified as: an integer value.

n columns number of submatrix belonging to blck to be inserted.

Scope:local.

Type:required.

Specified as: an integer value.

ix x global-row corresponding to position at which blck submatrix must be inserted.

Scope:local.

Type:required.

Specified as: an integer value.

jx x global-col corresponding to position at which blck submatrix must be inserted.

Scope:local.

Type:required.

Specified as: an integer value.

blck the dense submatrix to be inserted.

Scope:local.

Type:required.

Specified as: a one or two dimensional array.

desc_a the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

iblck first row of submatrix belonging to blck to be inserted.

Scope:local.

Type:required.

Specified as: an integer value.

jblck first column of submatrix belonging to blck to be inserted.

Scope:local.

Type:required.

Specified as: an integer value.

On Return

 \mathbf{x} the output dense matrix.

Scope: **local** Type: **required**

Specified as: a one or two dimensional array.

info Error code. Scope: local

Type: required

psb_sprn—Reinit sparse matrix structure for psblas routines.

Syntax

call psb_sprn (a, decsc_a, info)

On Entry

a the matrix to be reinitialized.

Scope:local

Type:required

Specified as: a structured data of type psb_spmat_type.

 $\mathbf{desc_a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

On Return

info Error code. Scope: local

Type: required

Specified as: an integer variable.

psb_glob_to_loc—Global to local indices convertion

Syntax

call psb_glob_to_loc (x, y, desc_a, info, iact)
call psb_glob_to_loc (x, desc_a, info, iact)

On Entry

 \mathbf{x} An integer vector of indices to be converted.

Scope: **local** Type: **required**

Specified as: a rank one integer array.

 $\mathbf{desc}_{-\mathbf{a}}$ the communication descriptor.

Scope: local.

Type:required.

Specified as: a structured data of type psb_desc_type.

iact specifies action to be taken in case of range errors. Scope: global

Type: **optional**

Specified as: a character variable E, W or A.

On Return

x If y is not present, then x is overwritten with the translated integer indices.

Scope: **global**Type: **required**

Specified as: a rank one integer array.

y If y is not present, then y is overwritten with the translated integer indices,

and x is left unchanged. Scope: global

Type: **optional**

Specified as: a rank one integer array.

info Error code. Scope: local

Type: **required**

Specified as: an integer variable.

psb_loc_to_glob—Local to global indices conversion

Syntax

call psb_loc_to_glob $(x, y, desc_a, info, iact)$ call psb_loc_to_glob $(x, desc_a, info, iact)$

On Entry

 \mathbf{x} An integer vector of indices to be converted.

Scope: **local**Type: **required**

Specified as: a rank one integer array.

 $\mathbf{desc}_{-}\mathbf{a}$ the communication descriptor.

Scope:local.

Type:required.

Specified as: a structured data of type psb_desc_type.

iact specifies action to be taken in case of range errors. Scope: global

Type: optional

Specified as: a character variable E, W or A.

On Return

 \mathbf{x} If y is not present, then x is overwritten with the translated integer indices.

Scope: **global**Type: **required**

Specified as: a rank one integer array.

y If y is not present, then y is overwritten with the translated integer indices,

and x is left unchanged. Scope: **global**

Type: **optional**

Specified as: a rank one integer array.

info Error code. Scope: local

Type: **required**

Specified as: an integer variable.

7 Iterative Methods

In this chapter we provide routines for preconditioners and iterative methods. Their interfaces are defined in the module <code>psb_methd_mod</code>

psb_cg —CG Iterative Method

This subroutine implements the CG method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\| + \|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_cgs $(a, prec, b, x, eps, desc_a, info, itmax, iter, err, itrace, istop)$

On Entry

 \mathbf{a} the local portion of global sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global**Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global** Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global**Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global**Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**

Type: **optional**Returned as: an integer variable.

psb_cgs —CGS Iterative Method

This subroutine implements the CGS method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\|+\|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_cgs $(a,prec,b,x,eps,desc_a,info,itmax,iter,err,itrace,istop)$

On Entry

 \mathbf{a} the local portion of global sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global**Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global** Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global**Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global** Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**

Type: **optional**Returned as: an integer variable.

psb_bicg —BiCG Iterative Method

This subroutine implements the BiCG method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\|+\|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_bicg $(a, prec, b, x, eps, desc_a, info, itmax, iter, err, itrace, istop)$

On Entry

 \mathbf{a} the local portion of global sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global**Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global** Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global**Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global**Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**

Type: **optional**Returned as: an integer variable.

psb_bicgstab —BiCGSTAB Iterative Method

This subroutine implements the BiCGSTAB method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\|+\|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_bicgstab $(a, prec, b, x, eps, desc_a, info, itmax, iter, err, itrace, istop)$

On Entry

 \mathbf{a} the local portion of global sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global** Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global** Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global** Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global**Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**

Type: **optional**Returned as: an integer variable.

${\bf psb_bicgstabl-BiCGSTAB-} l\ {\bf Iterative} \\ {\bf Method}$

This subroutine implements the BiCGSTAB-l method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\| + \|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_bicgstab $(a, prec, b, x, eps, desc_a, info, itmax, iter, err, itrace, irst, istop)$

On Entry

a the local portion of global sparse matrix A.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global**Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

irst An integer specifying the restarting iteration.

Scope: **global** Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global**Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global**Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global** Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**Type: **optional**

Returned as: an integer variable.

psb_gmres —GMRES Iterative Method

This subroutine implements the GMRES method with restarting. The stopping criterion is the normwise backward error, in the infinity norm, i.e. the iteration is stopped when

$$\frac{\|r\|}{(\|A\|\|x\|+\|b\|)} < eps$$

or

$$\frac{\|r_i\|}{\|b\|_2} < eps$$

according to the value passed through the istop argument (see later).

Syntax

call psb_gmres $(a, prec, b, x, eps, desc_a, info, itmax, iter, err, itrace, irst, istop)$

On Entry

 \mathbf{a} the local portion of global sparse matrix A.

Scope: **local**Type: **required**

Specified as: a structured data of type psb_spmat_type.

prec The data structure containing the preconditioner.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_prec_type.

b The RHS vector.

Scope: **local** Type: **required**

Specified as: a rank one array.

 \mathbf{x} The initial guess.

Scope: **local** Type: **required**

Specified as: a rank one array.

eps The stopping tolerance.

Scope: **global**Type: **required**

Specified as: a real number.

desc_a contains data structures for communications.

Scope: **local** Type: **required**

Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.

Scope: **global** Type: **optional**

Default: itmax = 1000.

Specified as: an integer variable $itmax \ge 1$.

itrace A tracing parameter.

Scope: **global**Type: **optional**

irst An integer specifying the restart iteration.

Scope: **global** Type: **optional**

istop An integer specifying the stopping criterion.

Scope: **global**Type: **optional**

On Return

 \mathbf{x} The computed solution.

Scope: **local**Type: **required**

Specified as: a rank one array.

iter The number of iterations performed.

Scope: **global** Type: **optional**

Returned as: an integer variable.

err The error estimate on exit.

Scope: **global** Type: **optional**

Returned as: a real number.

info An error code.

Scope: **global**Type: **optional**

Returned as: an integer variable.

8 Preconditioner routines

Preconditioning is somehow regarded as "black magic". This is due to the fact that theory doesn't provide a reliable support in the choice of a preconditioner. It is clear that the influence of a preconditioning technique on the convergence behavior of an iterative method mostly depends on the characteristics of the system matrix and of the method itself. Anyway it is not possible a priori to say that one preconditioner is algebrically better than another and this perfectly explains the importance of providing a wide range of preconditioners techniques so that the user can find by itself which one is more suitable for his problem. Moreover, there are some other issues to consider when choosing a preconditioner such as balancing the overhead of building the preconditioner with the reduction in the number of iterations. PSBLAS contains the implementation of many preconditioning techniques some of which are very flexible thanks to the presence of many parameters that is possible to adjust to fit the user's needs:

- Diagonal Scaling
- Block Jacobi with ILU(0) factorization
- Additive Schwarz with the Restricted Additive Schwarz and Additive Schwarz with Harmonic extensions (see chapter ??)
- Two-Level Additive Schwarz; this is actually a family of preconditioners since there is the possibility to choose between many variants as explained in chapter ??

psb_precset—Sets the precodntioner type

Syntax

```
call psb_precset (prec, ptype, iv, rs, rv, ierr)
```

On Entry

```
prec Scope: global
    Type: required
```

Specified as: e pronditioner data structure psb_prec_type.

ptype the type of preconditioner. Scope: global

Type: **required** Specified as: a string.

iv integer parameters for the precondtioner. Scope: global

Type: required

Specified as: an integer array.

rs Scope:

Type:

Specified as: .

rv Scope:

Type:

Specified as: .

ierr Scope:

Type:

Specified as: .

psb_precbld—Builds a preconditioner

Syntax

call psb_precbld (a, desc_a, prec, info, upd)

On Entry

a the system sparse matrix. Scope: global

Type: required

Specified as: a sparse matrix data structure psb_spmat_type.

desc_a the problem communication descriptor. Scope: global

Type: required

Specified as: a communication descriptor data structure psb_desc_type.

upd Scope: global

Type: **optional**

Specified as: a character.

On Return

prec the precodntioner.

Scope: **global**Type: **required**

Specified as: a precondtioner data structure psb_prec_type

info the return error code.

Scope: **local**Type: **required**

$psb_precaply — Preconditioner\ application$ routine

Syntax

call psb_precaply $(prec, x, y, desc_a, info, trans, work)$

Syntax

call psb_precaply $(prec, x, desc_a, info, trans)$

On Entry

prec the preconditioner. Scope: global

Type: **required**

Specified as: a preconditioner data structure psb_prec_type.

x the source vector. Scope: **global**

Type: require

Specified as: a double precision array.

desc_a the problem communication descriptor. Scope: global

Type: **required**

Specified as: a communication data structure psb_desc_type.

trans Scope:

Type: **optional**

Specified as: a character.

work an optional work space Scope: local

Type: **optional**

Specified as: a double precision array.

On Return

y the destination vector. Scope: global

Type: required

Specified as: a double precision array.

info the return error code.

Scope: **local** Type: **required**Specified as: an integer.

9 Error handling

The PSBLAS library error handling policy has been completely rewritten in version 2.0. The idea behind the design of this new error handling strategy is to keep error messages on a stack allowing the user to trace back up to the point where the first error message has been generated. Every routine in the PSBLAS-2.0 library has, as last non-optional argument, an integer info variable; whenever, inside the routine, en error is detected, this variable is set to a value corresponding to a specific error code. Then this error code is also pushed on the error stack and then either control is returned to the caller routine or the execution is aborted, depending on the users choice. At the time when the execution is aborted, an error message is printed on standard output with a level of verbosity than can be chosen by the user. If the execution is not aborted, then, the caller routine checks the value returned in the info variable and, if not zero, an error condition is raised. This process continues on all the levels of nested calls until the level where the user decides to abort the program execution.

Figure 5 shows the layout of a generic psb_foo routine with respect to the PSBLAS-2.0 error handling policy. It is possible to see how, whenever an error condition is detected, the info variable is set to the corresponding error code which is, then, pushed on top of the stack by means of the psb_errpush. An error condition may be directly detected inside a routine or indirectly checking the error code returned returned by a called routine. Whenever an error is encountered, after it has been pushed on stack, the program execution skips to a point where the error condition is handled; the error condition is handled either by returning control to the caller routine or by calling the psb_error routine which prints the content of the error stack and aborts the program execution.

Figure 6 reports a sample error message generated by the PSBLAS-2.0 library. This error has been generated by the fact that the user has chosen the invalid "FOO" storage format to represent the sparse matrix. From this error message it is possible to see that the error has been detected inside the psb_cest subroutine called by psb_spasb ... by process 0 (i.e. the root process).

```
subroutine psb_foo(some args, info)
   if(error detected) then
      info=errcode1
      call psb_errpush('psb_foo', errcode1)
      goto 9999
   end if
   call psb_bar(some args, info)
   if(info .ne. zero) then
      info=errcode2
      call psb_errpush('psb_foo', errcode2)
      goto 9999
   end if
9999 continue
   if (err_act .eq. act_abort) then
     call psb_error(icontxt)
     return
   else
     return
   end if
end subroutine psb_foo
```

Figure 5: The layout of a generic psb_foo routine with respect to PSBLAS-2.0 error handling policy.

Process: O. PSBLAS Error (4010) in subroutine: df_sample
Error from call to subroutine mat dist

Process: O. PSBLAS Error (4010) in subroutine: mat_distv
Error from call to subroutine psb_spasb

Process: O. PSBLAS Error (4010) in subroutine: psb_spasb
Error from call to subroutine psb_cest

Process: O. PSBLAS Error (4010) in subroutine: psb_spasb
Error from call to subroutine psb_cest

Process: O. PSBLAS Error (136) in subroutine: psb_cest
Format FOO is unknown

Aborting...

Figure 6: A sample PSBLAS-2.0 error message. Process 0 detected an error condition inside the psb_cest subroutine

$psb_errpush$ —Pushes an error code onto the error stack

Syntax

call psb_errpush (err_c, r_name, i_err, a_err)

On Entry

 $\mathbf{err}_{\mathbf{c}}$ the error code

Scope: **local** Type: **required**

Specified as: an integer.

r_name the soutine where the error has been caught.

Scope: **local**Type: **required**Specified as: a string.

 i_err addional info for error code

Scope: **local** Type: **optional**

Specified as: an integer array

 $\mathbf{a}_{-}\mathbf{err}$ addional info for error code

Scope: **local**Type: **optional**Specified as: a string.

psb_error —Prints the error stack content and aborts execution

Syntax

call psb_error (icontxt)

On Entry

icontxt the communication context.

Scope: **global**Type: **optional**

$psb_set_errverbosity$ —Sets the verbosity of error messages.

Syntax

call psb_set_err
verbosity (\emph{v})

On Entry

 ${f v}$ the verbosity level

Scope: **global**Type: **required**

psb_set_erraction—Set the type of action to be taken upon error condition.

Syntax

call $psb_set_erraction\ (err_act)$

On Entry

 ${\bf err_act}$ the type of action.

Scope: **global**Type: **required**

$psb_errcomm$ —Error communication routine

Syntax

call psb_errcomm (icontxt, err)

On Entry

icontxt the communication context.

Scope: **global**Type: **required**

Specified as: an integer.

err the error code to be communicated

Scope: **global**Type: **required**