PSBLAS-2.1 User's guide

A reference guide for the Parallel Sparse BLAS library

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Contents

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.

The PSBLAS library is internally implemented in a mixture of Fortran 77 and Fortran 95 [21] programming languages. A similar approach has been advocated by a number of authors, e.g. [20]. 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. In the current release we rely on the availability of the so-called allocatable extensions, specified in TR 15581. Strictly speaking they are outside the Fortran 95 standard; however they have been included in the Fortran 2003 language standard, and are available in prctically all Fortran 95 compilers on the market, including the GCC compiler from the Free Software Foundation (as of version 4.2). The presentation of the PSBLAS library follows the general structure of the proposal for serial Sparse BLAS [15, 16], which in its turn is based on the proposal for BLAS on dense matrices [1, 2, 3].

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 document will be discussed referring to a finite difference discretization of a Partial Differential Equation (PDE). 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. 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 [14] 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.

In any case we provide wrappers around the BLACS routines so that the user does not need to delve into their details (see Sec. 7).

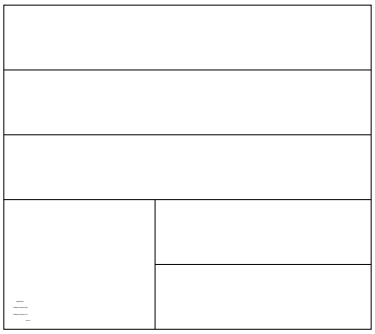

Figure 1: PSBLAS library components hierarchy.

The type of linear system matrices that we address typically arise in the numerical solution of PDEs; in such a context, it is necessary to pay special attention to the structure of the problem from which the application originates. The nonzero pattern of a matrix arising from the discretization of a PDE is influenced by various factors, such as the shape of the domain, the discretization strategy, and the equation/unknown ordering. The matrix itself can be interpreted as the adjacency matrix of the graph associated with the discretization mesh.

The distribution of the coefficient matrix for the linear system is based on the "owner computes" rule: the variable associated to each mesh point is assigned to a process that will own the corresponding row in the coefficient matrix and will carry out all related computations. This allocation strategy is equivalent to a

partition of the discretization mesh into *sub-domains*. Our library supports any distribution that keeps together the coefficients of each matrix row; there are no other constraints on the variable assignment. This choice is consistent with data distributions commonly used in ScaLAPACK such as `CYCLIC(N)` and `BLOCK`, as well as completely arbitrary assignments of equation indices to processes. In particular it is consistent with the usage of graph partitioning tools commonly available in the literature, e.g. METIS [19]. Dense vectors conform to sparse matrices, that is, the entries of a vector follow the same distribution of the matrix rows.

We assume that the sparse matrix is built in parallel, where each process generates its own portion. We never require that the entire matrix be available on a single node. However, it is possible to hold the entire matrix in one process and distribute it explicitly[1], even though the resulting bottleneck would make this option unattractive in most cases.

2.1 Basic Nomenclature

Our computational model implies that the data allocation on the parallel distributed memory machine is guided by the structure of the physical model, and specifically by the discretization mesh of the PDE.

Each point of the discretization mesh will have (at least) one associated equation/variable, and therefore one index. We say that point i *depends* on point j if the equation for a variable associated with i contains a term in j, or equivalently if $a_{ij} \neq 0$. After the partition of the discretization mesh into *sub-domains* assigned to the parallel processes, we classify the points of a given sub-domain as following.

Internal. An internal point of a given domain *depends* only on points of the same domain. If all points of a domain are assigned to one process, then a computational step (e.g., a matrix-vector product) of the equations associated with the internal points requires no data items from other domains and no communications.

Boundary. A point of a given domain is a boundary point if it *depends* on points belonging to other domains.

Halo. A halo point for a given domain is a point belonging to another domain such that there is a boundary point which *depends* on it. Whenever performing a computational step, such as a matrix-vector product, the values associated with halo points are requested from other domains. A boundary point of a given domain is a halo point for (at least) another domain; therefore the cardinality of the boundary points set denotes the amount of data sent to other domains.

Overlap. An overlap point is a boundary point assigned to multiple domains. Any operation that involves an overlap point has to be replicated for each assignment.

Overlap points do not usually exist in the basic data distribution, but they are a feature of Domain Decomposition Schwarz preconditioners which we are in the process of including in our distribution [6, 11].

[1] In our prototype implementation we provide sample scatter/gather routines.

We denote the sets of internal, boundary and halo points for a given subdomain by $\mathcal{I}$, $\mathcal{B}$ and $\mathcal{H}$. Each subdomain is assigned to one process; each process usually owns one subdomain, although the user may choose to assign more than one subdomain to a process. If each process i owns one subdomain, the number of rows in the local sparse matrix is $|\mathcal{I}_i| + |\mathcal{B}_i|$, and the number of local columns (i.e. those for which there exists at least one non-zero entry in the local rows) is $|\mathcal{I}_i| + |\mathcal{B}_i| + |\mathcal{H}_i|$.

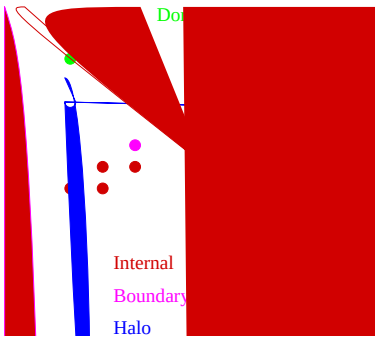

Figure 2: Point classfication.

This classification of mesh points guides the naming scheme that we adopted in the library internals and in the data structures. We explicitly note that "Halo" points are also often called "ghost" points in the literature.

2.2 Library contents

The PSBLAS library consists of various classes of subroutines:

Computational routines comprising:

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

Communication routines handling halo and overlap communications;

Data management and auxiliary routines including:

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

Preconditioner routines

Iterative methods a subset of Krylov subspace iterative methods

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:
  - `ge`: 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_geins`, `psb_spins` and `psb_cdins` perform the same action (see 6) 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.

In the description of the subroutines, arguments or argument entries are classified as:

global For input arguments, the value must be the same on all processes participating in the subroutine call; for output arguments the value is guaranteed to be the same.

local Each process has its own value(s) independently.

2.3 Application structure

The main underlying principle of the PSBLAS library is that the library objects are created and exist with reference to a discretized space to which there corresponds an index space and a matrix sparsity pattern. As an example, consider a cell-centered finite-volume discretization of the Navier-Stokes equations on a simulation domain; the index space $1 \ldots n$ is isomorphic to the set of cell centers, whereas the pattern of the associated linear system matrix is isomorphic to the adjacency graph imposed on the discretization mesh by the discretization stencil.

Thus the first order of business is to establish an index space, and this is done with a call to `psb_cdall` in which we specify the size of the index space n and the allocation of the elements of the index space to the various processes making up the MPI (virtual) parallel machine.

The index space is partitioned among processes, and this creates a mapping from the "global" numbering $1 \ldots n$ to a numbering "local" to each process; each process i will own a certain subset $1 \ldots n_{\mathrm{row}_i}$, each element of which corresponds to a certain element of $1 \ldots n$. The user does not set explicitly this mapping; when the application needs to indicate to which element of the index space a certain item is related, such as the row and column index of a matrix coefficient,

it does so in the "global" numbering, and the library will translate into the appropriate "local" numbering.

For a given index space $1 \ldots n$ there are many possible associated topologies, i.e. many different discretization stencils; thus the description of the index space is not completed until the user has defined a sparsity pattern, either explicitly through `psb_cdins` or implicitly through `psb_spins`. The descriptor is finalized with a call to `psb_cdasb` and a sparse matrix with a call to `psb_spasb`. After `psb_cdasb` each process i will have defined a set of "halo" (or "ghost") indices $n_{\mathrm{row}_i} + 1 \ldots n_{\mathrm{col}_i}$, denoting elements of the index space that are *not* assigned to process i; however the variables associated with them are needed to complete computations associated with the sparse matrix A, and thus they have to be fetched from (neighbouring) processes. The descriptor of the index space is built exactly for the purpose of properly sequencing the communication steps required to achieve this objective.

A simple application structure will walk through the index space allocation, matrix/vector creation and linear system solution as follows:

1. Initialize parallel environment with `psb_init`
2. Initialize index space with `psb_cdall`
3. Allocate sparse matrix and dense vectors with `psb_spall` and `psb_geall`
4. Loop over all local rows, generate matrix and vector entries, and insert them with `psb_spins` and `psb_geins`
5. Assemble the various entities:
   (a) `psb_cdasb`
   (b) `psb_spasb`
   (c) `psb_geasb`
6. Choose the preconditioner to be used with `psb_precset` and build it with `psb_precbld`
7. Call the iterative method of choice, e.g. `psb_bicgstab`

This is the structure of the sample program `test/pargen/ppde90.f90`.

For a simulation in which the same discretization mesh is used over multiple time steps, the following structure may be more appropriate:

1. Initialize parallel environment with `psb_init`
2. Initialize index space with `psb_cdall`
3. Loop over the topology of the discretization mesh and build the descriptor with `psb_cdins`
4. Assemble the descriptor with `psb_cdasb`
5. Allocate the sparse matrices and dense vectors with `psb_spall` and `psb_geall`
6. Loop over the time steps:

(a) If after first time step, reinitialize the sparse matrix with `psb_sprn`; also zero out the dense vectors;

(b) Loop over the mesh, generate the coefficients and insert/update them with `psb_spins` and `psb_geins`

(c) Assemble with `psb_spasb` and `psb_geasb`

(d) Choose and build preconditioner with `psb_precset` and `psb_precbld`

(e) Call the iterative method of choice, e.g. `psb_bicgstab`

The insertion routines will be called as many times as needed; they only need to be called on the data that is actually allocated to the current process, i.e. each process generates its own data.

In principle there is no specific order in the calls to `psb_spins`, nor is there a requirement to build a matrix row in its entirety before calling the routine; this allows the application programmer to walk through the discretization mesh element by element, generating the main part of a given matrix row but also contributions to the rows corresponding to neighbouring elements.

From a functional point of view it is even possible to execute one call for each nonzero coefficient; however this would have a substantial computational overhead. It is therefore advisable to pack a certain amount of data into each call to the insertion routine, say touching on a few tens of rows; the best performng value would depend on both the architecture of the computer being used and on the problem structure. At the opposite extreme, it would be possible to generate the entire part of a coefficient matrix residing on a process and pass it in a single call to `psb_spins`; this, however, would entail a doubling of memory occupation, and thus would be almost always far from optimal.

2.4 Programming model

The PSBLAS librarary is based on the Single Program Multiple Data (SPMD) programming model: each process participating in the computation performs the same actions on a chunk of data. Parallelism is thus data-driven.

Because of this structure, practically all subroutines *must* be called simultaneously by all processes participating in the computation, i.e each subroutine call acts implicitly as a synchronization point. The exceptions to this rule are:

- The insertion routines `psb_cdins`, `psb_spins` and `psb_geins`;
- The error handling routines.

In particular, as per the discussion in the previous section, the insertion routines may be called a different number of times on each process, depending on the data distribution chosen by the user.

3 Data Structures

In this chapter we illustrate the data structures used for definition of routines interfaces. They include data structures for sparse matrices, communication descriptors and preconditioners.

All the data types and subroutine interfaces are defined in the module `psb_base_mod`; this will have to be included by every user subroutine that makes use of the library.

3.1 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 a transparent mode by the tools routines of Sec. 6 while creating a new sparse matrix, and its fields may be accessed if necessary via appropriate routines; nevertheless we include its description for the curious reader:

matrix_data includes general information about matrix and process 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 associated with the processes comprised in the virtual parallel machine (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: an allocatable integer array of dimension `psb_mdata_size_`.

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: an allocatable 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: an allocatable integer array of rank one.

ovrlap_index For all overlap points belonging to th ecurrent 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: an allocatable integer array of rank one.

loc_to_glob each element i of this array contains global identifier of the local variable i.
Specified as: an allocatable integer array of rank one.

glob_to_loc if global variable i is read by current process then element i contains local index correpondent to global variable i; else element i contains -1 (NULL) value.
Specified as: an allocatabled integer array of rank one.

The Fortran95 definition for `psb_desc_type` structures is as follows:

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

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

A communication descriptor associated with a sparse matrix has a state, which can take the following values:

Build: State entered after the first allocation, and before the first assembly; in this state it is possible to add communication requirements among different processes.

Assembled: State entered after the assembly; computations using the associated sparse matrix, such as matrix-vector products, are only possible in this state.

3.1.1 Named Constants

psb_none_ Generic no-op;

psb_nohalo_ Do not fetch halo elements;

psb_halo_ Fetch halo elements from neighbouring processes;

psb_sum_ Sum overlapped elements

psb_avg_ Average overlapped elements

psb_dec_type_ Entry holding decomposition type (in `desc_a%matrix_data`)

psb_m_ Entry holding total number of rows

psb_n_ Entry holding total number of columns

psb_n_row_ Entry holding the number of rows stored in the current process

psb_n_col_ Entry holding the number of columns stored in the current process

psb_ctxt_ Entry holding a copy of the BLACS communication context

psb_desc_asb_ State of the descriptor: assembled, i.e. suitable for computational tasks.

psb_desc_bld_ State of the descriptor: build, must be assembled before computational use.

3.2 Sparse Matrix data structure

The `psb_spmat_type` data structure contains all information about local portion of the sparse matrix and its storage mode. Most of these fields are set by the tools routines when inserting a new sparse matrix; the user needs only choose, if he/she so whishes, a specific matrix storage mode.

aspk Contains values of the local distributed sparse matrix.
Specified as: an allocatable 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: an allocatable integer array of rank one.

ia2 Holds integer information on distributed sparse matrix. Actual information will depend on data format used.
Specified as: an allocatable 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: an integer array of length `psb_ifasize_`.

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: an allocatable 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 columnm permutation.
Specified as: an allocatable 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.

FORTRAN95 interface for distributed sparse matrices containing double precision real entries is defined as in figure 4.

```
type psb_dspmat_type
   integer     :: m, k
   character   :: fida(5)
   character   :: descra(10)
   integer     :: infoa(psb_ifa_size_)
   real(kind(1.d0)), allocatable :: aspk(:)
   integer, allocatable :: ia1(:), ia2(:)
   integer, allocatable :: pr(:), pl(:)
end type psb_dspmat_type
```

Figure 4: 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 $ia2(1) \leq j \leq ia2(m+1)-1$.

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 $1 \leq j \leq infoa(1)$, the coefficient, row index and column index are stored into `apsk(j)`, `ia1(j)` and `ia2(j)` respectively.

A sparse matrix has an associated state, which can take the following values:

Build: State entered after the first allocation, and before the first assembly; in this state it is possible to add nonzero entries.

Assembled: State entered after the assembly; computations using the sparse matrix, such as matrix-vector products, are only possible in this state;

Update: State entered after a reinitalization; this is used to handle applications in which the same sparsity pattern is used multiple times with different coefficients. In this state it is only possible to enter coefficients for already existing nonzero entries.

3.2.1 Named Constants

psb_dupl_ovwrt_ Duplicate coefficients should be overwritten (i.e. ignore duplications)

psb_dupl_add_ Duplicate coefficients should be added;

psb_dupl_err_ Duplicate coefficients should trigger an error conditino

psb_upd_dflt_ Default update strategy for matrix coefficients;

psb_upd_srch_ Update strategy based on search into the data structure;

psb_upd_perm_ Update strategy based on additional permutation data (see tools routine description).

3.3 Preconditioner data structure

Our library offers support for many different types of preconditioning schemes. Besides the simple well known preconditioners like Diagonal Scaling or Block Jacobi with either incomplete factorization ILU(0) or complete LU factorization. We also provide an experimental package of complex preconditioning methods like the Additive Schwarz and Multilevel Additive Schwarz; these last preconditioners will be described in a separate document.

A preconditioner is held in the psb_prec_type data structure which depends on the psb_base_prec reported in figure 5. 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_precbld subroutine. This data structure wants to be flexible enough to easily allow the implementation of new kind of preconditioners. The values contained in the iprcparm and dprcparm 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_dbaseprc_type

  type(psb_dspmat_type), allocatable :: av(:)
  real(kind(1.d0)), allocatable      :: d(:)
  type(psb_desc_type)                :: desc_data , desc_ac
  integer, allocatable               :: iprcparm(:)
  real(kind(1.d0)), allocatable      :: dprcparm(:)
  integer, allocatable               :: perm(:),  invperm(:)
  integer, allocatable               :: mlia(:), nlaggr(:)
  type(psb_dspmat_type), pointer     :: base_a    => null() !
  type(psb_desc_type), pointer       :: base_desc => null() !
  real(kind(1.d0)), allocatable      :: dorig(:)

end type psb_dbaseprc_type

type psb_dprec_type
  type(psb_dbaseprc_type), allocatable  :: baseprecv(:)
  integer                         :: prec, base_prec
end type psb_dprec_type
```

Figure 5: The PSBLAS defined data type that contains a preconditioner.

3.3.1 Named Constants

f_ilu_n_ Incomplete LU factorization with n levels of fill-in; currently only $n = 0$ is implemented;

f_slu_ Sparse factorization using SuperLU;

f_umf_ Sparse factorization using UMFPACK;

add_ml_prec_ Additive multilevel correction;

mult_ml_prec_ Multiplicative multilevel correction;

pre_smooth_ Pre-smoothing in applying multiplicative multilevel corrections;

post_smooth_ Post-smoothing in applying multiplicative multilevel corrections;

smooth_both_ Two-sided (i.e. symmetric) smoothing in applying multiplicative multilevel corrections;

mat_distr_ Coarse matrix distributed among processes

mat_repl_ Coarse matrix replicated among processes

4 Computational routines

psb_geaxpby—General Dense Matrix Sum

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

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

Syntax

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

x, y, α, β	**Subroutine**
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.

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.

y the local portion of the global dense matrix y.
Scope: **local**
Type: **required**
Specified as: a rank one or two array containing numbers of the type indicated in Table 1. 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

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**
An integer value that contains an error code.

psb_gedot—Dot Product

This function computes dot product between two vectors x and y.
If x and y are double 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:

$$dot \leftarrow x^H y$$

Syntax

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

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

Table 2: Data types

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: an 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.
Scope: **local**
Type: **required**
Specified as: an 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`.

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**
An integer value that contains an error code.

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**
Long Precision Real	psb_gedot
Long Precision Complex	psb_gedot

Table 3: Data types

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: an array of rank one or two containing numbers of type specified in Table 3. The rank of x must be the same of y.

y the local portion of global dense matrix y.
Scope: **local**
Type: **required**
Specified as: an 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: **global**
Specified as: a number or a rank-one array of the data type indicated in Table 2.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

psb_geamax—Infinity-Norm of Vector

This function computes the infinity-norm of a vector x.
If x is a double precision real vector computes infinity norm as:

$$amax \leftarrow \max_i |x_i|$$

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

$$amax \leftarrow \max_i (|re(x_i)| + |im(x_i)|)$$

Syntax

psb_geamax (x, *desc_a*, *info*)

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

Table 4: Data types

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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`.

On Return

Function value is the infinity norm of subvector x.
Scope: **global**
Specified as: a long precision real number.

info Scope: **global**
Type: **required**
An integer value that contains an error code.

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**
Long Precision Real	Long Precision Real	psb_geamax
Long Precision Real	Long Precision Complex	psb_geamax

Table 5: Data types

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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 long precision real numbers.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

psb_geasum—1-Norm of Vector

This function computes the 1-norm of a vector x.
If x is a double precision real vector computes 1-norm as:

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

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

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

Syntax

psb_geasum (*x, desc_a, info*)

asum	*x*	**Function**
Long Precision Real	Long Precision Real	psb_geasum
Long Precision Real	Long Precision Complex	psb_geasum

Table 6: Data types

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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`.

On Return

Function value is the 1-norm of vector x.
Scope: **global**
Specified as: a long precision real number.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

psb_genrm2—2-Norm of Vector

This function computes the 2-norm of a vector x.
If x is a double precision real vector computes 2-norm as:

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

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

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

$nrm2$	x	**Function**
Long Precision Real	Long Precision Real	psb_genrm2
Long Precision Real	Long Precision Complex	psb_genrm2

Table 7: Data types

Syntax

psb_genrm2 (x, *desc_a*, *info*)

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.

On Return

Function Value is the 2-norm of subvector x.
Scope: **global**
Type: **required**
Specified as: a long precision real number.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

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

A	**Function**
Long Precision Real	psb_spnrmi
Long Precision Complex	psb_spnrmi

Table 8: Data types

Syntax

psb_spnrmi (A, *desc_a*, *info*)

On Entry

a the local portion of the global sparse matrix A.
Scope: **local**
Type: **required**
Specified as: a structured data of type psb_spmat_type.

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 long precision real number.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

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 $x_{:,:}$

y is the global dense submatrix $y_{:,:}$

A is the global sparse submatrix A

P_r, P_c are the permutation matrices.

A, x, y, α, β	**Subroutine**
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, work*)

On Entry

alpha the scalar α.
Scope: **global**
Type: **required**
Specified as: a number of the data type indicated in Table 9.

a the local portion of the sparse matrix A.
Scope: **local**
Type: **required**
Specified as: a structured data of type `psb_spmat_type`.

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.

work work array.
Scope: **local**
Type: **optional**
Specified as: a rank one array of the same type of x and y with the TARGET attribute.

On Return

y the local portion of result submatrix y.
Scope: **local**
Type: **required**
Specified as: an array of rank one or two containing numbers of type specified in Table 9.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

psb_spsm—Triangular System Solve

This subroutine computes the Triangular System Solve:

$$
\begin{aligned}
y &\leftarrow \alpha P_r T^{-1} P_c x + \beta y \\
y &\leftarrow \alpha D P_r T^{-1} P_c x + \beta y \\
y &\leftarrow \alpha P_r T^{-1} P_c D x + \beta y \\
y &\leftarrow \alpha P_r T^{-T} P_c x + \beta y \\
y &\leftarrow \alpha D P_r T^{-T} P_c x + \beta y \\
y &\leftarrow \alpha P_r T^{-T} P_c D x + \beta y \\
y &\leftarrow \alpha P_r T^{-H} P_c x + \beta y \\
y &\leftarrow \alpha D P_r T^{-H} P_c x + \beta y \\
y &\leftarrow \alpha P_r T^{-H} P_c D x + \beta y
\end{aligned}
$$

where:

x is the global dense submatrix $x_{:,:}$

y is the global dense submatrix $y_{:,:}$

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, work*)

T, x, y, D, α, β	**Subroutine**
Long Precision Real	psb_spsm
Long Precision Complex	psb_spsm

Table 10: Data types

On Entry

alpha the scalar α.
Scope: **global**
Type: **required**
Specified as: a number of the data type indicated in Table 10.

t the global portion of the sparse matrix T.
Scope: **local**
Type: **required**
Specified as: a structured data type specified in § 3.

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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 specifies the update of overlap elements to be performed on exit:

`psb_none_`

`psb_sum_`

`psb_avg_`

`psb_square_root_`

Scope: **global**
Type: **optional**
Default: `psb_avg_`
Specified as: an integer 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.

work a work array.
Scope: **local**
Type: **optional**
Specified as: a rank one array of the same type of x with the TARGET attribute.

On Return

y the local portion of global dense matrix y.
Scope: **local**
Type: **required**
Specified as: an array of rank one or two containing numbers of type specified in Table 10.

info Scope: **local**
Type: **required**
An integer value that contains an error code.

5 Communication routines

The routines in this chapter implement various global communication operators on vectors associated with a discretization mesh. For auxiliary communication routines not tied to a discretization space see 6.

psb_halo—Halo Data Communication

These subroutines gathers the values of the halo elements, and (optionally) scale the result:

$$x \leftarrow \alpha x$$

where:

x is a global dense submatrix.

α, x	**Subroutine**
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

x global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the TARGET 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

x global dense result matrix x.
Scope: **local**
Type: **required**
Returned as: a rank one or two array 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 applies an overlap operator to the input vector:

$$x \leftarrow Qx$$

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.

x	**Subroutine**
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, update=update_type, work=work*)

On Entry

x global dense matrix x.
Scope: **local**
Type: **required**
Specified as: a rank one or two array 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.

update Update operator.

update = psb_none_ Do nothing;
update = psb_add_ Sum overlap entries, i.e. apply P^T;
update = psb_avg_ Average overlap entries, i.e. apply $P_a P^T$;

Scope: **global**
Default: *update_type = psb_avg_*
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

x global dense result matrix x.
Scope: **local**
Type: **required**
Specified as: an 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 associated with the descriptor, no operations are performed;

2. The operator P^T performs the reduction sum of overlap elements; it is a "prolongation" operator P^T 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.

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**
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 $0 \leq ix \leq np$.

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 $1 \leq ix \leq matrix\_data(psb\_m\_)$.

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**
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 $0 \leq ix \leq np$.

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 $1 \leq ix \leq matrix\_data(psb\_m\_)$.

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 routines

psb_cdall—Allocates a communication descriptor

Syntax

call psb_cdall (*icontxt, desc_a, info,mg,parts*)

Syntax

call psb_cdall (*icontxt, desc_a, info,vg,flag*)

Syntax

call psb_cdall (*icontxt, desc_a, info,vl*)

This subroutine initializes the communication descriptor associated with an index space. Exactly one of the optional arguments `parts`, `vg`, `vl` must be specified, thereby choosing the specific initialization strategy:

On Entry

icontxt the communication context.
Scope:**global**.
Type:**required**.
Specified as: an integer value.

vg Data allocation: each index $i \in \{1 \dots mg\}$ is allocated to process $vg(i)$.
Scope:**global**.
Type:**optional**.
Specified as: an integer array.

flag Specifies whether entries in vg are zero- or one-based. Scope:**global**.
Type:**optional**.
Specified as: an integer value $0, 1$, default 0.

mg the (global) number of rows of the problem.
Scope:**global**.
Type:**optional**.
Specified as: an integer value. It is required if `parts` is specified.

parts the subroutine that defines the partitioning scheme.
Scope:**global**.
Type:**required**.
Specified as: a subroutine.

vl Data allocation: the set of global indices belonging to the calling process.
Scope:**local**.
Type:**optional**.
Specified as: an integer array.

On Return

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. Exactly one of the optional arguments `parts`, `vg`, `vl` must be specified, thereby choosing the initialization strategy as follows:

   parts In this case we have a subroutine that takes as input a index and the total number of indices in the space, and produces in output a vector containing the set of processes (usually with just one entry) to which the index should be assigned. If this argument is specified, then it is mandatory to also specify the argument `mg`.

   vg In this case the association between an index and a process is specified via an integer vector; the size of the index space is equal to the size of `vg`, and each index i is assigned to the process $vg(i)$. The vector `vg` must be identical on all calling processes; its entries may have the ranges $(0 \ldots np-1)$ or $(1 \ldots np)$ according to the value of `flag`.

   vl In this case we are specifying the list of indices assigned to the current process; thus, the global problem size mg is given by the sum of the sizes of the individual vectors `vl` specified on the calling processes. The subroutine will check that each entry in the global index space $(1 \ldots mg)$ is specified exactly once.

2. On exit from this routine the descriptor is in the build state

psb_cdins—Communication descriptor insert routine

Syntax

call psb_cdins (*nz, ia, ja, desc_a, info*)

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.

On Return

desc_a the updated communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type `psb_desc_type`.

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. This routine may only be called if the descriptor is in the build state

psb_cdasb—Communication descriptor assembly routine

Syntax

call psb_cdasb (*desc_a, info*)

On Entry

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.

Notes

1. On exit from this routine the descriptor is in the assembled state.

psb_cdcpy—Copies a communication descriptor

Syntax

call psb_cdcpy (*desc_out, desc_a, info*)

On Entry

desc_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**
Specified as: an integer variable.

psb_cdfree—Frees a communication descriptor

Syntax

call psb_cdfree (*desc_a, info*)

On Entry

desc_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**
Specified as: an integer variable.

psb_spall—Allocates a sparse matrix

Syntax

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

On Entry

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

nnz An estimate of the number of nonzeroes in the local part of the assembled 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**
Specified as: an integer variable.

Notes

1. On exit from this routine the sparse matrix is in the build state.
2. The descriptor may be in either the build or assembled state.
3. Providing a good estimate for the number of nonzeroes *nnz* in the assembled matrix may substantially improve performance in the matrix build phase, as it will reduce or eliminate the need for (potentially multiple) data reallocations.

psb_spins—Insert a cloud of elements into a sparse matrix

Syntax

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

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.

desc_a The communication descriptor.
Scope: **local**.
Type: **required**.
Specified as: a variable of type psb_desc_type.

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.

desc_a The communication descriptor.
Scope: **local**.
Type: **required**.
Specified as: a variable of type psb_desc_type.

info Error code.
Scope: **local**
Type: **required**

Notes

1. On entry to this routine the descriptor may be in either the build or assembled state.
2. On entry to this routine the sparse matrix may be in either the build or update state.
3. If the descriptor is in the build state, then the sparse matrix ought also be in the build state; the action of the routine is to (implicitly) call `psb_cdins` to add entries to the sparsity pattern;
4. If the descriptor is in the assembled state, then any entries in the sparse matrix that would generate additional communication requirements will be ignored;
5. If the matrix is in the update state, any entries in positions that were not present in the original matrix will be ignored.

psb_spasb—Sparse matrix assembly routine

Syntax

call psb_spasb (*a, desc_a, info, afmt, upd, dupl*)

On Entry

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

afmt the storage format for the sparse matrix.
Scope: **global**.
Type: **optional**.
Specified as: an array of characters. Defalt: 'CSR'.

upd Provide for updates to the matrix coefficients.
Scope: **global**.
Type: **optional**.
Specified as: integer, possible values: `psb_upd_srch_`, `psb_upd_perm_`

dupl How to handle duplicate coefficients.
Scope: **global**.
Type: **optional**.
Specified as: integer, possible values: `psb_dupl_ovwrt_`, `psb_dupl_add_`, `psb_dupl_err_`.

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**
Specified as: an integer variable.

Notes

1. On entry to this routine the descriptor must be in the assembled state, i.e. `psb_cdasb` must already have been called.
2. The sparse matrix may be in either the build or update state;
3. Duplicate entries are detected and handled in both build and update state, with the exception of the error action that is only taken in the build state, i.e. on the first assembly;

4. If the update choice is `psb_upd_perm_`, then subsequent calls to `psb_spins` to update the matrix must be arranged in such a way as to produce exactly the same sequence of coefficient values as encountered at the first assembly;
5. On exit from this routine the matrix is in the assembled state, and thus is suitable for the computational routines.

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.

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_sprn—Reinit sparse matrix structure for psblas routines.

Syntax

call psb_sprn (*a, decsc_a, info, clear*)

On Entry

a the matrix to be reinitialized.
Scope:**local**
Type:**required**
Specified as: a structured data of type psb_spmat_type.

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

clear Choose whether to zero out matrix coefficients
Scope:**local**.
Type:**optional**.
Default: true.

On Return

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. On exit from this routine the sparse matrix is in the update state.

psb_geall—Allocates a dense matrix

Syntax

call psb_geall (x, *desc_a*, *info*, n)

On Entry

desc_a The communication descriptor.
Scope: **local**
Type: **required**
Specified as: a variable of type psb_desc_type.

n The number of columns of the dense matrix to be allocated.
Scope: **local**
Type: **optional**
Specified as: Integer scalar, default 1. It is ignored if x is a rank-1 array.

On Return

x The dense matrix to be allocated.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the ALLOCATABLE attribute, of type real, complex or integer.

info Error code. Scope: **local**
Type: **required**
Specified as: Integer scalar.

psb_geins—Dense matrix insertion routine

Syntax

call psb_geins (*m, irw, val, x, desc_a, info,dupl*)

On Entry

m Number of rows in *val* to be inserted.
Scope:**local**.
Type:**required**.
Specified as: an integer value.

irw Indices of the rows to be inserted. Specifically, row i of *val* will be inserted into the local row corresponding to the global row index $irw(i)$.
Scope:**local**.
Type:**required**.
Specified as: an integer array.

val the dense submatrix to be inserted.
Scope:**local**.
Type:**required**.
Specified as: a rank 1 or 2 array. Specified as: an integer value.

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type `psb_desc_type`.

dupl How to handle duplicate coefficients.
Scope: **global**.
Type: **optional**.
Specified as: integer, possible values: `psb_dupl_ovwrt_`, `psb_dupl_add_`.

On Return

x the output dense matrix.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the ALLOCATABLE attribute, of type real, complex or integer.

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. Dense vectors/matrices do not have an associated state;
2. Duplicate entries are either overwritten or added, there is no provision for raising an error condition.

psb_geasb—Assembly a dense matrix

Syntax

call psb_geasb (*x, desc_a, info*)

On Entry

desc_a The communication descriptor.
Scope: **local**
Type: **required**
Specified as: a variable of type psb_desc_type.

On Return

x The dense matrix to be assembled.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the ALLOCATABLE attribute, of type real, complex or integer.

info Error code.
Scope: **local**
Type: **required**
Specified as: Integer scalar.

psb_gefree—Frees a dense matrix

Syntax

call psb_gefree (*x, desc_a, info*)

On Entry

x The dense matrix to be freed.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the ALLOCATABLE attribute, of type real, complex or integer.

desc_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**
Specified as: Integer scalar.

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.

x The dense matrix to be permuted.
Scope: **local**
Type: **required**
Specified as: a one or two dimensional array.

desc_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**
Specified as: Integer scalar.

psb_glob_to_loc—Global to local indices convertion

Syntax

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

call psb_glob_to_loc (*x, desc_a, info, iact,owned*)

On Entry

x An integer vector of indices to be converted.
Scope: **local**
Type: **required**
Specified as: a rank one integer array.

desc_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 `Ignore`, `Warning` or `Abort`, default `Ignore`.

owned Specfies valid range of input Scope: **global**
Type: **optional**
If true, then only indices strictly owned by the current process are considered valid, if false then halo indices are also accepted. Default: false.

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 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.

Notes

1. If an input index is out of range, then the corresponding output index is set to a negative number;
2. The default `Ignore` means that the negative output is the only action taken on an out-of-range input.

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

x An integer vector of indices to be converted.
Scope: **local**
Type: **required**
Specified as: a rank one integer array.

desc_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_geall—Allocates a dense matrix

Syntax

call psb_geall (*x, desc_a, info, n*)

On Entry

desc_a The communication descriptor.
Scope: **local**
Type: **required**
Specified as: a variable of type psb_desc_type.

n The number of columns of the dense matrix to be allocated.
Scope: **local**
Type: **optional**
Specified as: Integer scalar, default 1. It is ignored if x is a rank-1 array.

On Return

x The dense matrix to be allocated.
Scope: **local**
Type: **required**
Specified as: a rank one or two array with the ALLOCATABLE attribute, of type real, complex or integer.

info Error code. Scope: **local**
Type: **required**
Specified as: Integer scalar.

psb_get_boundary—Extract list of boundary elements

Syntax

call psb_get_boundary (*bndel, desc, info*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

bndel The list of boundary elements on the calling process, in local numbering.
Scope: **local**
Type: **required**
Specified as: a rank one array with the ALLOCATABLE attribute, of type integer.

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. If there are no boundary elements (i.e., if the local part of the connectivity graph is self-contained) the output vector is set to `NULL()`
2. Otherwise the size of `bndel` will be exactly equal to the number of boundary elements.

psb_get_overlap—Extract list of overlap elements

Syntax

call psb_get_overlap (*ovrel, desc, info*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

ovrel The list of overlap elements on the calling process, in local numbering.
Scope: **local**
Type: **required**
Specified as: a rank one array with the ALLOCATABLE attribute, of type integer.

info Error code. Scope: **local**
Type: **required**
Specified as: an integer variable.

Notes

1. If there are no overlap elements the output vector is set to `NULL()`
2. Otherwise the size of `ovrel` will be exactly equal to the number of overlap elements.

psb_cd_get_local_rows—Get number of local rows

Syntax

nr = psb_cd_get_local_rows (*desc*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

Function value The number of local rows, i.e. the number of rows owned by the current process; as explained in 1, it is equal to $|\mathcal{I}_i| + |\mathcal{B}_i|$. The returned value is specific to the calling process.

psb_cd_get_local_cols—Get number of local cols

Syntax

nc = psb_cd_get_local_cols (*desc*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

Function value The number of local cols, i.e. the number of indices used by the current process, including both local and halo indices; as explained in 1, it is equal to $|\mathcal{I}_i| + |\mathcal{B}_i| + |\mathcal{H}_i|$. The returned value is specific to the calling process.

psb_cd_get_global_rows—Get number of global rows

Syntax

nr = psb_cd_get_global_rows (*desc*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

Function value The number of global rows in the mesh

psb_cd_get_contex—Get communication context

Syntax

ictxt = psb_cd_get_context (*desc*)

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Specified as: a structured data of type psb_desc_type.

On Return

Function value The communication context.

psb_sp_get_nrows—Get number of rows in a sparse matrix

Syntax

nr = psb_sp_get_nrows (a)

On Entry

a the sparse matrix
Scope:**local**
Type:**required**
Specified as: a structured data of type psb_spmat_type.

On Return

Function value The number of rows of sparse matrix a.

psb_sp_get_ncols—Get number of columns in a sparse matrix

Syntax

nr = psb_sp_get_ncols (a)

On Entry

a the sparse matrix
Scope:**local**
Type:**required**
Specified as: a structured data of type psb_spmat_type.

On Return

Function value The number of columns of sparse matrix a.

psb_sp_get_nnzeros—Get number of nonzero elements in a sparse matrix

Syntax

nr = psb_sp_get_nnzeros (a)

On Entry

a the sparse matrix
Scope:**local**
Type:**required**
Specified as: a structured data of type psb_spmat_type.

On Return

Function value The number of nonzero elements stored in sparse matrix a.

Notes

1. The function value is specific to the storage format of matrix a; some storage formats employ padding, thus the returned value for the same matrix may be different for different storage choices.

7 Parallel environment routines

psb_init—Initializes PSBLAS parallel environment

Syntax

call psb_init (*icontxt, np*)

This subroutine initializes the PSBLAS parallel environment, defining a virtual parallel machine.

On Entry

np Number of processes in the PSBLAS virtual parallel machine.
Scope:**global**.
Type:**optional**.
Specified as: an integer value. Default: use all available processes provided by the underlying parallel environment.

On Return

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

Notes

1. A call to this routine must precede any other PSBLAS call.
2. It is an error to specify a value for *np* greater than the number of processes available in the underlying parallel execution environment.

psb_info—Return information about PSBLAS parallel environment

Syntax

call psb_info (*icontxt, iam, np*)

This subroutine returns informantion about the PSBLAS parallel environment, defining a virtual parallel machine.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

On Return

iam Identifier of current process in the PSBLAS virtual parallel machine.
Scope:**local**.
Type:**required**.
Specified as: an integer value. $-1 \leq iam \leq np-1$

np Number of processes in the PSBLAS virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

Notes

1. For processes in the virtual parallel machine the identifier will satisfy $0 \leq iam \leq np-1$;
2. If the user has requested on `psb_init` a number of processes less than the total available in the parallel execution environment, the remaining processes will have on return $iam = -1$; the only call involving `icontxt` that any such process may execute is to `psb_exit`.

psb_exit—Exit from PSBLAS parallel environment

Syntax

call psb_exit (*icontxt*)

call psb_exit (*icontxt,close*)

This subroutine exits from the PSBLAS parallel virtual machine.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

close Whether to close all data structures related to the virtual parallel machine, besides those associated with icontxt.
Scope:**global**.
Type:**optional**.
Specified as: a logical variable, default value: true.

Notes

1. This routine may be called even if a previous call to `psb_info` has returned with $iam = -1$; indeed, it it is the only routine that may be called with argument `icontxt` in this situation.

2. If the user wants to use multiple communication contexts in the same program, this routine may be called multiple times to selectively close the contexts with `close=.false.`, while on the last call it should be called with `close=.true.` to shutdown in a clean way the entire parallel environment.

psb_get_mpicomm—Get the MPI communicator

Syntax

call psb_get_mpicomm (*icontxt, icomm*)

This subroutine returns the MPI communicator associated with a PSBLAS context

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

On Return

icomm The MPI communicator associated with the PSBLAS virtual parallel machine.
Scope:**global**.
Type:**required**.

psb_get_rank—Get the MPI rank

Syntax

call psb_get_rank (*rank, icontxt, id*)

This subroutine returns the MPI rank of the PSBLAS process *id*

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

id Identifier of a process in the PSBLAS virtual parallel machine.
Scope:**local**.
Type:**required**.
Specified as: an integer value. $0 \leq id \leq np - 1$

On Return

rank The MPI rank associated with the PSBLAS process *id*.
Scope:**local**.
Type:**required**.

psb_wtime—Wall clock timing

Syntax

time = psb_wtime ()

This function returns a wall clock timer. The resolution of the timer is dependent on the underlying parallel environment implementation.

On Exit

Function value the elapsed time in seconds.
Returned as: a `real(kind(1.d0))` integer variable.

psb_barrier—Sinchronization point parallel environment

Syntax

call psb_barrier (*icontxt*)

This subroutine acts as a synchronization point for the PSBLAS parallel virtual machine. As such, it must be called by all participating processes.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

psb_abort—Abort a computation

Syntax

call psb_abort (*icontxt*)

This subroutine aborts computation on the parallel virtual machine.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

psb_bcast—Broadcast data

Syntax

call psb_bcast (*icontxt, dat, root*)

This subroutine implements a broadcast operation based on the underlying communication library.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

dat On the root process, the data to be broadcast.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array, or a character or logical scalar. Type, rank and size must agree on all processes.

root Root process holding data to be broadcast.
Scope:**global**.
Type:**optional**.
Specified as: an integer value $0 <= root <= np - 1$, default 0

On Return

dat On processes other than root, the data to be broadcast.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array, or a character or logical scalar. Type, rank and size must agree on all processes.

psb_sum—Global sum

Syntax

call psb_sum (*icontxt, dat, root*)

This subroutine implements a sum reduction operation based on the underlying communication library.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

dat The local contribution to the global sum.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, rank and size must agree on all processes.

root Process to hold the final sum, or -1 to make it available on all processes.
Scope:**global**.
Type:**optional**.
Specified as: an integer value $-1 <= root <= np - 1$, default -1.

On Return

dat On destination process(es), the result of the sum operation.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array.
Type, rank and size must agree on all processes.

Notes

1. The `dat` argument is both input and output, and its value may be changed even on processes different from the final result destination.

psb_amx—Global maximum absolute value

Syntax

call psb_amx (*icontxt, dat, root*)

This subroutine implements a maximum absolute value reduction operation based on the underlying communication library.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

dat The local contribution to the global maximum.
Scope:**local**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, rank and size must agree on all processes.

root Process to hold the final sum, or -1 to make it available on all processes.
Scope:**global**.
Type:**optional**.
Specified as: an integer value $-1 <= root <= np - 1$, default -1.

On Return

dat On destination process(es), the result of the maximum operation.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, rank and size must agree on all processes.

Notes

1. The `dat` argument is both input and output, and its value may be changed even on processes different from the final result destination.

psb_amn—Global minimum absolute value

Syntax

call psb_amn (*icontxt, dat, root*)

This subroutine implements a minimum absolute value reduction operation based on the underlying communication library.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

dat The local contribution to the global minimum.
Scope:**local**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, rank and size must agree on all processes.

root Process to hold the final sum, or -1 to make it available on all processes.
Scope:**global**.
Type:**optional**.
Specified as: an integer value $-1 <= root <= np - 1$, default -1.

On Return

dat On destination process(es), the result of the minimum operation.
Scope:**global**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array.
Type, rank and size must agree on all processes.

Notes

1. The `dat` argument is both input and output, and its value may be changed even on processes different from the final result destination.

psb_snd—Send data

Syntax

call psb_snd (*icontxt, dat, dst, m*)

This subroutine sends a packet of data to a destination.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

dat The data to be sent.
Scope:**local**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array, or a character or logical scalar. Type and rank must agree on sender and receiver process; if m is not specified, size must agree as well.

dst Destination process.
Scope:**global**.
Type:**required**.
Specified as: an integer value $0 <= dst <= np - 1$.

m Number of rows.
Scope:**global**.
Type:**Optional**.
Specified as: an integer value $0 <= m <= size(dat, 1)$.
When *dat* is a rank 2 array, specifies the number of rows to be sent independently of the leading dimension $size(dat, 1)$; must have the same value on sending and receiving processes.

On Return

psb_rcv—Receive data

Syntax

call psb_rcv (*icontxt, dat, src, m*)

This subroutine receives a packet of data to a destination.

On Entry

icontxt the communication context identifying the virtual parallel machine.
Scope:**global**.
Type:**required**.
Specified as: an integer variable.

src Source process.
Scope:**global**.
Type:**required**.
Specified as: an integer value $0 <= src <= np - 1$.

m Number of rows.
Scope:**global**.
Type:**Optional**.
Specified as: an integer value $0 <= m <= size(dat, 1)$.
When *dat* is a rank 2 array, specifies the number of rows to be sent independently of the leading dimension $size(dat, 1)$; must have the same value on sending and receiving processes.

On Return

dat The data to be received.
Scope:**local**.
Type:**required**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array, or a character or logical scalar. Type and rank must agree on sender and receiver process; if m is not specified, size must agree as well.

8 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 6 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 7 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 6: The layout of a generic `psb_foo` routine with respect to PSBLAS-2.0 error handling policy.

```
============================================================
Process: 0.  PSBLAS Error (4010) in subroutine: df_sample
Error from call to subroutine mat dist
============================================================
Process: 0.  PSBLAS Error (4010) in subroutine: mat_distv
Error from call to subroutine psb_spasb
============================================================
Process: 0.  PSBLAS Error (4010) in subroutine: psb_spasb
Error from call to subroutine psb_cest
============================================================
Process: 0.  PSBLAS Error (136) in subroutine: psb_cest
Format FOO is unknown
============================================================
Aborting...
```

Figure 7: 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

err_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

a_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**
Specified as: an integer.

psb_set_errverbosity—Sets the verbosity of error messages.

Syntax

call psb_set_errverbosity (v)

On Entry

v the verbosity level
Scope: **global**
Type: **required**
Specified as: an integer.

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

Syntax

call psb_set_erraction (*err_act*)

On Entry

err_act the type of action.
Scope: **global**
Type: **required**
Specified as: an integer.

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**
Specified as: an integer.

9 Preconditioner routines

The base PSBLAS library contains the implementation of two simple preconditioning techniques:

- Diagonal Scaling
- Block Jacobi with ILU(0) factorization

The supporting data type and subroutine interfaces are defined in the module `psb_prec_mod`.

psb_precset—Sets the preconditioner type

Syntax

call psb_precset (*prec, ptype, info*)

On Entry

prec Scope: **local**
Type: **required**
Specified as: a pronditioner data structure psb_prec_type.

ptype the type of preconditioner. Scope: **global**
Type: **required**
Specified as: a character string, see usage notes.

On Exit

info Scope: **global**
Type: **required**
Error code: if no error, 0 is returned.

Usage Notes

Legal inputs to this subroutine are interpreted depending on the *ptype* string as follows[2]:

NONE No preconditioning, i.e. the preconditioner is just a copy operator.

DIAG Diagonal scaling; each entry of the input vector is multiplied by the reciprocal of the sum of the absolute values of the coefficients in the corresponding row of matrix A;

ILU, BJA Precondition by the incomplete LU factorization of the block-diagonal of matrix A, where block boundaries are determined by the data allocation boundaries for each process; requires no communication. Only $ILU(0)$ is currently implemented.

[2]The string is case-insensitive

psb_precbld—Builds a preconditioner

Syntax

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

On Entry

a the system sparse matrix. Scope: **local**
Type: **required**
Specified as: a sparse matrix data structure `psb_spmat_type`.

desc_a the problem communication descriptor. Scope: **local**
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 preconditioner.
Scope: **local**
Type: **required**
Specified as: a precondtioner data structure `psb_prec_type`

info the return error code.
Scope: **global**
Type: **required**
Specified as: an integer, upon successful completion $info = 0$

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: **local**
Type: **required**
Specified as: a preconditioner data structure psb_prec_type.

x the source vector. Scope: **local**
Type: **require**
Specified as: a double precision array.

desc_a the problem communication descriptor. Scope: **local**
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: **local**
Type: **required**
Specified as: a double precision array.

info the return error code.
Scope: **local**
Type: **required**
Specified as: an integer, upon successful completion $info = 0$.

psb_prec_descr—Prints a description of current preconditioner

Syntax

call psb_prec_descr (*prec*)

On Entry

prec the preconditioner. Scope: **local**
Type: **required**
Specified as: a preconditioner data structure psb_prec_type.

10 Iterative Methods

In this chapter we provide routines for preconditioners and iterative methods.

psb_krylov —Krylov Methods Driver Routine

This subroutine is a driver that provides a general interface for all the Krylov-Subspace family methods implemented in PSBLAS-2.0. 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_krylov (*method,a,prec,b,x,eps,desc_a,info,itmax,iter,err,itrace,istop*)

On Entry

method a string that defines the iterative method to be used. Valid values in PSBLAS-2.0 are:

CG : the Conjugate gradient method;

CGS :the Conjugate Gradient Stabilized method;

BICG : the Bi-Conjugate Gradient method;

BICGSTAB : the Bi-Conjugate Gradient Stabilized method;

BICGSTABL : the Bi-Conjugate Gradient Stabilized method with restarting;

RGMRES : the Generalized Minimal Residual method with restarting.

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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every $itrace$ iterations.
Scope: **global**
Type: **optional**

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**

On Return

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_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_cg (*a,prec,b,x,eps,desc_a,info,itmax,iter,err,itrace,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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every $itrace$ iterations.
Scope: **global**
Type: **optional**

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**

On Return

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

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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every $itrace$ iterations.
Scope: **global**
Type: **optional**

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**

On Return

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

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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every $itrace$ iterations.
Scope: **global**
Type: **optional**

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**

On Return

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

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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every $itrace$ iterations.
Scope: **global**
Type: **optional**

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**

On Return

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_bicgstabl —BiCGSTAB-l Iterative 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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every *itrace* iterations.
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

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

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.

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 $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every *itrace* iterations.
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

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.

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