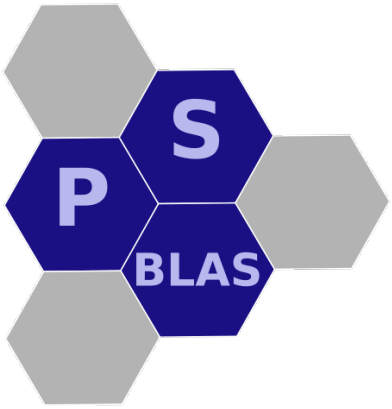
PSBLAS 3.9.0 User's guide

A reference guide for the Parallel Sparse BLAS library



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1 Introduction

The PSBLAS library, developed with the aim to facilitate the parallelization of computationally intensive scientific applications, is designed to address parallel implementation of iterative solvers for sparse linear systems through the distributed memory paradigm. It includes routines for multiplying sparse matrices by dense matrices, solving block diagonal systems with triangular diagonal entries, preprocessing sparse matrices, and contains additional routines for dense matrix operations. The current implementation of PSBLAS addresses a distributed memory execution model operating with message passing.

The PSBLAS library version 3 is implemented in the Fortran 2003 [17] programming language, with reuse and/or adaptation of existing Fortran 77 and Fortran 95 software, plus a handful of C routines.

The use of Fortran 2003 offers a number of advantages over Fortran 95, mostly in the handling of requirements for evolution and adaptation of the library to new computing architectures and integration of new algorithms. For a detailed discussion of our design see [11]; other works discussing advanced programming in Fortran 2003 include [21, 19]; sufficient support for Fortran 2003 is now available from many compilers, including the GNU Fortran compiler from the Free Software Foundation (as of version 4.8).

Previous approaches have been based on mixing Fortran 95, with its support for object-based design, with other languages; these have been advocated by a number of authors, e.g. [16]. Moreover, the Fortran 95 facilities for dynamic memory management and interface overloading greatly enhance the usability of the PSBLAS subroutines. In this way, the library can take care of runtime memory requirements that are quite difficult or even impossible to predict at implementation or compilation time.

The presentation of the PSBLAS library follows the general structure of the proposal for serial Sparse BLAS [8, 9], which in its turn is based on the proposal for BLAS on dense matrices [15, 5, 6].

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 solutions to these problems and other important inputs to the development of the PSBLAS software package

have 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 2003 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 encapsulated in an applicaiton layer that has been strongly inspired by the Basic Linear Algebra Communication Subroutines (BLACS) library [7]. Usually there is no need to deal directly with MPI; however, in some cases, MPI routines are used directly to improve efficiency. For further details on our communication layer see Sec. 7.

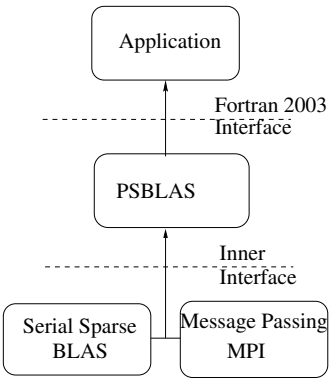

Figure 1: PSBLAS library components hierarchy.

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 simple data distributions 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 [14]. 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 memory 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 usually a halo point for some other domain[2]; therefore the cardinality of the boundary points set denotes the amount of data sent to other domains.

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

[2] This is the normal situation when the pattern of the sparse matrix is symmetric, which is equivalent to say that the interaction between two variables is reciprocal. If the matrix pattern is non-symmetric we may have one-way interactions, and these could cause a situation in which a boundary point is not a halo point for its neighbour.

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 distributions; however they are a feature of Domain Decomposition Schwarz preconditioners which are the subject of related research work [4, 3].

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 $|\mathcal{I}_i| + |\mathcal{B}_i| + |\mathcal{H}_i|$.

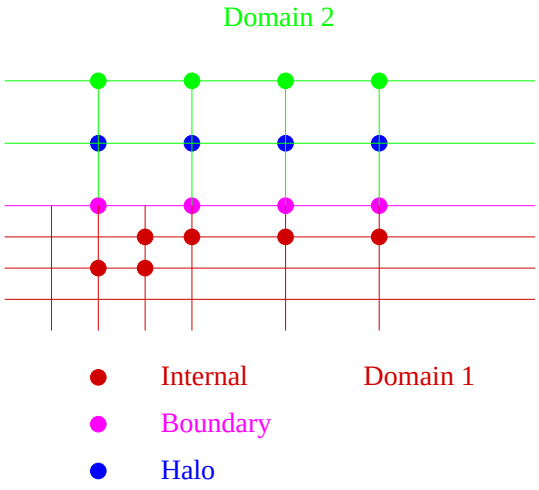

Figure 2: Point classfication.

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 symbols (i.e. subroutine names, data types...) are prefixed by `psb_`
- all data type names are suffixed by `_type`
- all constants are suffixed by `_`
- all top-level 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 names 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.

To finish our general description, we define a version string with the constant

`psb_version_string_`

whose current value is `3.9.0`

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 `prec%init` and `prec%set`, and build it with `prec%build`[3];
7. Call one of the iterative drivers with the method of choice, e.g. `psb_krylov` with `bicgstab`.

This is the structure of the sample programs in the directory `test/pargen/`.

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)
   (e) Choose the preconditioner to be used with `prec%init` and `prec%set`, and build it with `prec%build`;
   (f) Call one of the iterative drivers with the method of choice, e.g. `psb_krylov` with `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.

[3]The subroutine style `psb_precinit` and `psb_precbld` are still supported for backward compatibility

2.3.1 User-defined index mappings

PSBLAS supports user-defined global to local index mappings, subject to the constraints outlined in sec. 2.3:

1. The set of indices owned locally must be mapped to the set $1 \ldots n_{\mathrm{row}_i}$;
2. The set of halo points must be mapped to the set $n_{\mathrm{row}_i} + 1 \ldots n_{\mathrm{col}_i}$;

but otherwise the mapping is arbitrary. The user application is responsible to ensure consistency of this mapping; some errors may be caught by the library, but this is not guaranteed. The application structure to support this usage is as follows:

1. Initialize index space with `psb_cdall(ictx,desc,info,vl=vl,lidx=lidx)` passing the vectors `vl(:)` containing the set of global indices owned by the current process and `lidx(:)` containing the corresponding local indices;
2. Add the halo points `ja(:)` and their associated local indices `lidx(:)` with a(some) call(s) to `psb_cdins(nz,ja,desc,info,lidx=lidx)`;
3. Assemble the descriptor with `psb_cdasb`;
4. Build the sparse matrices and vectors, optionally making use in `psb_spins` and `psb_geins` of the `local` argument specifying that the indices in `ia`, `ja` and `irw`, respectively, are already local indices.

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, many subroutines coordinate their action across the various processes, thus providing an implicit synchronization point, and therefore *must* be called simultaneously by all processes participating in the computation. This is certainly true for the data allocation and assembly routines, for all the computational routines and for some of the tools routines.

However there are many cases where no synchronization, and indeed no communication among processes, is implied; for instance, all the routines in sec. 3 are only acting on the local data structures, and thus may be called independently. The most important case is that of the coefficient insertion routines: since the number of coefficients in the sparse and dense matrices varies among the processors, and since the user is free to choose an arbitrary order in builiding the matrix entries, these routines cannot imply a synchronization.

Throughout this user's guide each subroutine will be clearly indicated as:

Synchronous: must be called simultaneously by all the processes in the relevant communication context;

Asynchronous: may be called in a totally independent manner.

3 Data Structures and Classes

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 the basic subroutine interfaces related to descriptors and sparse matrices are defined in the module `psb_base_mod`; this will have to be included by every user subroutine that makes use of the library. The preconditioners are defined in the module `psb_prec_mod`

Integer, real and complex data types are parametrized with a kind type defined in the library as follows:

psb_spk_ Kind parameter for short precision real and complex data; corresponds to a `REAL` declaration and is normally 4 bytes;

psb_dpk_ Kind parameter for long precision real and complex data; corresponds to a `DOUBLE PRECISION` declaration and is normally 8 bytes;

psb_mpk_ Kind parameter for 4-bytes integer data, as is always used by MPI;

psb_epk_ Kind parameter for 8-bytes integer data, as is always used by the `sizeof` methods;

psb_ipk_ Kind parameter for "local" integer indices and data; with default build options this is a 4 bytes integer;

psb_lpk_ Kind parameter for "global" integer indices and data; with default build options this is an 8 bytes integer;

The integer kinds for local and global indices can be chosen at configure time to hold 4 or 8 bytes, with the global indices at least as large as the local ones. Together with the classes attributes we also discuss their methods. Most methods detailed here only act on the local variable, i.e. their action is purely local and asynchronous unless otherwise stated. The list of methods here is not completely exhaustive; many methods, especially those that alter the contents of the various objects, are usually not needed by the end-user, and therefore are described in the developer's documentation.

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 with a discretization pattern and enables data communications and other operations that are necessary for implementing the various algorithms of interest to us.

The data structure itself `psb_desc_type` can be treated as an opaque object handled via the tools routines of Sec. 6 or the query routines detailed below; nevertheless we include here a description for the curious reader.

First we describe the `psb_indx_map` type. This is a data structure that keeps track of a certain number of basic issues such as:

- The value of the communication context;

- The number of indices in the index space, i.e. global number of rows and columns of a sparse matrix;
- The local set of indices, including:
  - The number of local indices (and local rows);
  - The number of halo indices (and therefore local columns);
  - The global indices corresponding to the local ones.

There are many different schemes for storing these data; therefore there are a number of types extending the base one, and the descriptor structure holds a polymorphic object whose dynamic type can be any of the extended types. The methods associated with this data type answer the following queries:

- For a given set of local indices, find the corresponding indices in the global numbering;
- For a given set of global indices, find the corresponding indices in the local numbering, if any, or return an invalid
- Add a global index to the set of halo indices;
- Find the process owner of each member of a set of global indices.

All methods but the last are purely local; the last method potentially requires communication among processes, and thus is a synchronous method. The choice of a specific dynamic type for the index map is made at the time the descriptor is initially allocated, according to the mode of initialization (see also 6).

The descriptor contents are as follows:

indxmap A polymorphic variable of a type that is any extension of the indx_map type described above.

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;

Specified as: a vector of integer type, see 3.3.

ext_index A list of element indices to be exchanged to implement the mapping between a base descriptor and a descriptor with overlap.
Specified as: a vector of integer type, see 3.3.

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;

Specified as: a vector of integer type, see 3.3.

ovr_mst_idx A list to retrieve the value of each overlap element from the respective master process.
Specified as: a vector of integer type, see 3.3.

ovrlap_elem For all overlap points belonging to th ecurrent process:

1. Overlap point index;
2. Number of processes sharing that overlap points;
3. Index of a "master" process:

Specified as: an allocatable integer array of rank two.

bnd_elem A list of all boundary points, i.e. points that have a connection with other processes.

The Fortran 2003 declaration for `psb_desc_type` structures is as follows: A

```
type psb_desc_type
    class(psb_indx_map), allocatable :: indxmap
    type(psb_i_vect_type) :: v_halo_index
    type(psb_i_vect_type) :: v_ext_index
    type(psb_i_vect_type) :: v_ovrlap_index
    type(psb_i_vect_type) :: v_ovr_mst_idx
    integer, allocatable  :: ovrlap_elem(:,:)
    integer, allocatable  :: bnd_elem(:)
end type psb_desc_type
```

Listing 1: The PSBLAS defined data type that contains the communication descriptor.

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 Descriptor Methods

3.1.2 get_local_rows — Get number of local rows

```
nr = desc%get_local_rows()
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

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.

3.1.3 get_local_cols — Get number of local cols

```
nc = desc%get_local_cols()
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

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.

3.1.4 get_global_rows — Get number of global rows

```
nr = desc%get_global_rows()
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

On Return

Function value The number of global rows, i.e. the size of the global index space.

3.1.5 get_global_cols — Get number of global cols

```
nr = desc%get_global_cols()
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

On Return

Function value The number of global cols; usually this is equal to the number of global rows.

3.1.6 get_global_indices — Get vector of global indices

```
myidx = desc%get_global_indices([owned])
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.
Type: **required**.

owned Choose if you only want owned indices (`owned=.true.`) or also halo indices (`owned=.false.`). Scope: **local**.
Type: **optional**; default: `.true.`.

On Return

Function value The global indices, returned as an allocatable integer array of kind `psb_lpk_` and rank 1.

3.1.7 get_context — Get communication context

```
ctxt = desc%get_context()
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

On Return

Function value The communication context.

3.1.8 Clone — clone current object

```
call  desc%clone(descout,info)
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

On Return

descout A copy of the input object.

info Return code.

3.1.9 CNV — convert internal storage format

```
call  desc%cnv(mold)
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope: **local**.

mold the desired integer storage format.
Scope: **local**.
Specified as: a object of type derived from (integer) `psb_T_base_vect_type`.

The `mold` arguments may be employed to interface with special devices, such as GPUs and other accelerators.

3.1.10 psb_cd_get_large_threshold — Get threshold for index mapping switch

```
ith = psb_cd_get_large_threshold()
```

Type: Asynchronous.

On Return

Function value The current value for the size threshold.

3.1.11 psb_cd_set_large_threshold — Set threshold for index mapping switch

```
call psb_cd_set_large_threshold(ith)
```

Type: Synchronous.

On Entry

ith the new threshold for communication descriptors.
Scope: **global**.
Type: **required**.
Intent: **in**.
Specified as: an integer value greater than zero.

Note: the threshold value is only queried by the library at the time a call to `psb_cdall` is executed, therefore changing the threshold has no effect on communication descriptors that have already been initialized. Moreover the threshold must have the same value on all processes.

3.1.12 get_p_adjcncy — Get process adjacency list

```
list =  desc%get_p_adjcncy()
```

Type: Asynchronous.

On Return

Function value The current list of adjacent processes, i.e. processes with which the current one has to exchange halo data.

3.1.13 set_p_adjcncy — Set process adjacency list

```
call desc%set_p_adjcncy(list)
```

Type: Asynchronous.

On Entry

list the list of adjacent processes.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: a one-dimensional array of integers of kind `psb_ipk_`.

Note: this method can be called after a call to `psb_cdall` and before a call to `psb_cdasb`. The user is specifying here some knowledge about which processes are topological neighbours of the current process. The availability of this information may speed up the execution of the assembly call `psb_cdasb`.

3.1.14 fnd_owner — Find the owner process of a set of indices

```
call desc%fnd_owner(idx,iprc,info)
```

Type: Synchronous.

On Entry

idx the list of global indices for which we need the owning processes.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: a one-dimensional array of integers of kind `psb_lpk_`.

On Return

iprc the list of processes owning the indices in `idx`.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: an allocatable one-dimensional array of integers of kind `psb_ipk_`.

Note: this method may or may not actually require communications, depending on the exact internal data storage; given that the choice of storage may be altered by runtime parameters, it is necessary for safety that this method is called by all processes.

3.1.15 Named Constants

psb_none_ Generic no-op;

psb_root_ Default root process for broadcast and scatter operations;

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_comm_halo_ Exchange data based on the `halo_index` list;

psb_comm_ext_ Exchange data based on the `ext_index` list;

psb_comm_ovr_ Exchange data based on the `ovrlap_index` list;

psb_comm_mov_ Exchange data based on the `ovr_mst_idx` list;

3.2 Sparse Matrix class

The `psb_Tspmat_type` class contains all information about the local portion of the sparse matrix and its storage mode. Its design is based on the STATE design pattern [13] as detailed in [11]; the type declaration is shown in figure 2 where `T` is a placeholder for the data type and precision variants

S Single precision real;

D Double precision real;

C Single precision complex;

Z Double precision complex;

LS,LD,LC,LZ Same numeric type as above, but with `psb_lpk_` integer indices.

```
type :: psb_Tspmat_type
  class(psb_T_base_sparse_mat), allocatable  :: a
end type  psb_Tspmat_type
```

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

The actual data is contained in the polymorphic component `a%a` of type `psb_T_base_sparse_mat`; its specific layout can be chosen dynamically among the predefined types, or an entirely new storage layout can be implemented and passed to the library at runtime via the `psb_spasb` routine. The following very common formats are precompiled in PSBLAS and thus are always available:

psb_T_coo_sparse_mat Coordinate storage;

psb_T_csr_sparse_mat Compressed storage by rows;

psb_T_csc_sparse_mat Compressed storage by columns;

The inner 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.

The only storage variant supporting the build state is COO; all other variants are obtained by conversion to/from it.

3.2.1 Sparse Matrix Methods

3.2.2 get_nrows — Get number of rows in a sparse matrix

```
nr = a%get_nrows()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value The number of rows of sparse matrix `a`.

3.2.3 get_ncols — Get number of columns in a sparse matrix

```
nc = a%get_ncols()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value The number of columns of sparse matrix a.

3.2.4 get_nnzeros — Get number of nonzero elements in a sparse matrix

```
nz = a%get_nnzeros()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

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.

3.2.5 get_size — Get maximum number of nonzero elements in a sparse matrix

```
maxnz = a%get_size()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value The maximum number of nonzero elements that can be stored in sparse matrix a using its current memory allocation.

3.2.6 sizeof — Get memory occupation in bytes of a sparse matrix

```
memory_size = a%sizeof()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value The memory occupation in bytes.

3.2.7 get_fmt — Short description of the dynamic type

```
write(*,*) a%get_fmt()
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value A short string describing the dynamic type of the matrix. Predefined values include `NULL`, `COO`, `CSR` and `CSC`.

3.2.8 is_bld, is_upd, is_asb — Status check

```
if (a%is_bld()) then
if (a%is_upd()) then
if (a%is_asb()) then
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value A `logical` value indicating whether the matrix is in the Build, Update or Assembled state, respectively.

3.2.9 is_lower, is_upper, is_triangle, is_unit — Format check

```
if (a%is_triangle()) then
if (a%is_upper()) then
if (a%is_lower()) then
if (a%is_unit()) then
```

Type: Asynchronous.

On Entry

a the sparse matrix
Scope: **local**

On Return

Function value A `logical` value indicating whether the matrix is triangular; if `is_triangle()` returns `.true.` check also if it is lower, upper and with a unit (i.e. assumed) diagonal.

3.2.10 cscnv — Convert to a different storage format

```
call  a%cscnv(b,info [, type, mold, dupl])
call  a%cscnv(info [, type, mold, dupl])
```

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

type a string requesting a new format.
Type: optional.

mold a variable of `class(psb_T_base_sparse_mat)` requesting a new format.
Type: optional.

dupl an integer value specifing how to handle duplicates (see Named Constants below)

On Return

b,a A copy of `a` with a new storage format.
A variable of type `psb_Tspmat_type`.

info Return code.

The `mold` arguments may be employed to interface with special devices, such as GPUs and other accelerators.

3.2.11 csclip — Reduce to a submatrix

```
call a%csclip(b,info[,&
   & imin,imax,jmin,jmax,rscale,cscale])
```

Returns the submatrix `A(imin:imax,jmin:jmax)`, optionally rescaling row/-col indices to the range `1:imax-imin+1,1:jmax-jmin+1`.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

imin,imax,jmin,jmax Minimum and maximum row and column indices.
Type: optional.

rscale,cscale Whether to rescale row/column indices. Type: optional.

On Return

b A copy of a submatrix of `a`.
A variable of type `psb_Tspmat_type`.

info Return code.

3.2.12 clean_zeros — Eliminate zero coefficients

```
call a%clean_zeros(info)
```

Eliminates zero coefficients explicitly stored in the input matrix.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

On Return

a The matrix `a` without zero coefficients.
A variable of type `psb_Tspmat_type`.

info Return code.

Notes

1. Depending on the internal storage format, there may still be some amount of zero padding in the output.
2. Any explicit zeros on the main diagonal are always kept in the data structure.

3.2.13 get_diag — Get main diagonal

```
call a%get_diag(d,info)
```
Returns a copy of the main diagonal.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

On Return

d A copy of the main diagonal.
A one-dimensional array of the appropriate type.

info Return code.

3.2.14 clip_diag — Cut out main diagonal

```
call a%clip_diag(b,info)
```
Returns a copy of `a` without the main diagonal.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

On Return

b A copy of `a` without the main diagonal.
A variable of type `psb_Tspmat_type`.

info Return code.

3.2.15 tril — Return the lower triangle

```
call a%tril(l,info[,&
   & diag,imin,imax,jmin,jmax,rscale,cscale,u])
```

Returns the lower triangular part of submatrix `A(imin:imax,jmin:jmax)`, optionally rescaling row/col indices to the range `1:imax-imin+1,1:jmax-jmin+1` and returing the complementary upper triangle.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

diag Include diagonals up to this one; `diag=1` means the first superdiagonal, `diag=-1` means the first subdiagonal. Default 0.

imin,imax,jmin,jmax Minimum and maximum row and column indices.
Type: optional.

rscale,cscale Whether to rescale row/column indices. Type: optional.

On Return

l A copy of the lower triangle of `a`.
A variable of type `psb_Tspmat_type`.

u (optional) A copy of the upper triangle of `a`.
A variable of type `psb_Tspmat_type`.

info Return code.

3.2.16 triu — Return the upper triangle

```
call a%triu(u,info[,&
   & diag,imin,imax,jmin,jmax,rscale,cscale,l])
```

Returns the upper triangular part of submatrix `A(imin:imax,jmin:jmax)`, optionally rescaling row/col indices to the range `1:imax-imin+1,1:jmax-jmin+1`, and returing the complementary lower triangle.

Type: Asynchronous.

On Entry

a the sparse matrix.
A variable of type `psb_Tspmat_type`.
Scope: **local**.

diag Include diagonals up to this one; `diag=1` means the first superdiagonal, `diag=-1` means the first subdiagonal. Default 0.

imin,imax,jmin,jmax Minimum and maximum row and column indices.
Type: optional.

rscale,cscale Whether to rescale row/column indices. Type: optional.

On Return

u A copy of the upper triangle of `a`.
A variable of type `psb_Tspmat_type`.

l (optional) A copy of the lower triangle of `a`.
A variable of type `psb_Tspmat_type`.

info Return code.

3.2.17 psb_set_mat_default — Set default storage format

```
call  psb_set_mat_default(a)
```

Type: Asynchronous.

On Entry

a a variable of `class(psb_T_base_sparse_mat)` requesting a new default storage format.
Type: required.

3.2.18 clone — Clone current object

```
call  a%clone(b,info)
```

Type: Asynchronous.

On Entry

a the sparse matrix.
Scope: **local**.

On Return

b A copy of the input object.

info Return code.

3.2.19 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 Dense Vector Data Structure

The `psb_T_vect_type` data structure encapsulates the dense vectors in a way similar to sparse matrices, i.e. including a base type `psb_T_base_vect_type`. The user will not, in general, access the vector components directly, but rather via the routines of sec. 6. Among other simple things, we define here an extraction method that can be used to get a full copy of the part of the vector stored on the local process.

The type declaration is shown in figure 3 where `T` is a placeholder for the data type and precision variants

I Integer;

S Single precision real;

D Double precision real;

C Single precision complex;

Z Double precision complex.

The actual data is contained in the polymorphic component v%v; the separation between the application and the actual data is essential for cases where it is necessary to link to data storage made available elsewhere outside the direct control of the compiler/application, e.g. data stored in a graphics accelerator's private memory.

```
type psb_T_base_vect_type
  TYPE(KIND_), allocatable :: v(:)
end type psb_T_base_vect_type

type psb_T_vect_type
  class(psb_T_base_vect_type), allocatable :: v
end type  psb_T_vect_type
```

Listing 3: The PSBLAS defined data type that contains a dense vector.

3.3.1 Vector Methods

3.3.2 get_nrows — Get number of rows in a dense vector

```
nr = v%get_nrows()
```

Type: Asynchronous.

On Entry

v the dense vector
Scope: **local**

On Return

Function value The number of rows of dense vector v.

3.3.3 sizeof — Get memory occupation in bytes of a dense vector

```
memory_size = v%sizeof()
```

Type: Asynchronous.

On Entry

v the dense vector
Scope: **local**

On Return

Function value The memory occupation in bytes.

3.3.4 set — Set contents of the vector

```
call  v%set(alpha[,first,last])
call  v%set(vect[,first,last])
call  v%zero()
```

Type: Asynchronous.

On Entry

v the dense vector
Scope: **local**

alpha A scalar value.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 1.

first,last Boundaries for setting in the vector.
Scope: **local**
Type: **optional**
Intent: **in**.
Specified as: integers.

vect An array
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 1.

Note that a call to `v%zero()` is provided as a shorthand, but is equivalent to a call to `v%set(zero)` with the `zero` constant having the appropriate type and kind.

On Return

v the dense vector, with updated entries
Scope: **local**

3.3.5 get_vect — Get a copy of the vector contents

```
extv = v%get_vect([n])
```

Type: Asynchronous.

On Entry

v the dense vector
Scope: **local**

n Size to be returned
Scope: **local**.
Type: **optional**; default: entire vector.

On Return

Function value An allocatable array holding a copy of the dense vector contents. If the argument n is specified, the size of the returned array equals the minimum between n and the internal size of the vector, or 0 if n is negative; otherwise, the size of the array is the same as the internal size of the vector.

3.3.6 clone — Clone current object

```
call  x%clone(y,info)
```

Type: Asynchronous.

On Entry

x the dense vector.
Scope: **local**.

On Return

y A copy of the input object.

info Return code.

3.4 Preconditioner data structure

Our base library offers support for simple well known preconditioners like Diagonal Scaling or Block Jacobi with incomplete factorization ILU(0).

A preconditioner is held in the psb_Tprec_type data structure reported in figure 4. The psb_Tprec_type data type may contain a simple preconditioning matrix with the associated communication descriptor. The internal preconditioner is allocated appropriately with the dynamic type corresponding to the desired preconditioner.

```
type psb_Tprec_type
  class(psb_T_base_prec_type), allocatable :: prec
end type psb_Tprec_type
```

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

3.5 Heap data structure

Among the tools routines of sec. 6, we have a number of sorting utilities; the heap sort is implemented in terms of heaps having the following signatures:

`psb_T_heap` : a heap containing elements of type T, where T can be `i,s,c,d,z` for integer, real and complex data;

`psb_T_idx_heap` : a heap containing elements of type T, as above, together with an integer index.

Given a heap object, the following methods are defined on it:

init Initialize memory; also choose ascending or descending order;

howmany Current heap occupancy;

insert Add an item (or an item and its index);

get_first Remove and return the first element;

dump Print on file;

free Release memory.

These objects are used to implement the factorization and approximate inversion algorithms.

4 Computational routines

4.1 psb_geaxpby — General Dense Matrix Sum

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

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

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

x, y, α, β	**Subroutine**
Short Precision Real	psb_geaxpby
Long Precision Real	psb_geaxpby
Short Precision Complex	psb_geaxpby
Long Precision Complex	psb_geaxpby

Table 1: Data types

Type: Synchronous.

On Entry

alpha the scalar α.
Scope: **global**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**
Intent: **in**.
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**
Intent: **inout**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**

Intent: **in**.
Specified as: an object of type psb_desc_type.

On Return

y the local portion of result submatrix y.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type psb_T_vect_type containing numbers of the type indicated in Table 1.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.2 psb_gedot — Dot Product

This function computes dot product between two vectors x and y.
If x and y are real vectors it computes dot-product as:

$$dot \leftarrow x^T y$$

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

$$dot \leftarrow x^H y$$

```
psb_gedot(x, y, desc_a, info [,global])
```

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

Table 2: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**
Intent: **in**.
Specified as: an object of type psb_desc_type.

global Specifies whether the computation should include the global reduction across all processes.
Scope: **global**
Type: **optional**.

Intent: **in**.
Specified as: a logical scalar. Default: `global=.true.`

On Return

Function value is the dot product of vectors x and y.
Scope: **global** unless the optional variable `global=.false.` has been specified
Specified as: a number of the data type indicated in Table 2.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. The computation of a global result requires a global communication, which entails a significant overhead. It may be necessary and/or advisable to compute multiple dot products at the same time; in this case, it is possible to improve the runtime efficiency by using the following scheme:

```
vres(1) = psb_gedot(x1,y1,desc_a,info,global=.false.)
vres(2) = psb_gedot(x2,y2,desc_a,info,global=.false.)
vres(3) = psb_gedot(x3,y3,desc_a,info,global=.false.)
call psb_sum(ctxt,vres(1:3))
```

   In this way the global communication, which for small sizes is a latency-bound operation, is invoked only once.

4.3 psb_gedots — 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.

```
call psb_gedots(res, x, y, desc_a, info)
```

res, *x*, *y*	**Subroutine**
Short Precision Real	psb_gedots
Long Precision Real	psb_gedots
Short Precision Complex	psb_gedots
Long Precision Complex	psb_gedots

Table 3: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type 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**
Intent: **in**.
Specified as: an object of type psb_desc_type.

On Return

res is the dot product of vectors x and y.
Scope: **global**
Intent: **out**.
Specified as: a number or a rank-one array of the data type indicated in Table 2.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.4 psb_normi — Infinity-Norm of Vector

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

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

else if x is a complex vector then it computes the infinity-norm as:

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

```
   psb_geamax(x, desc_a, info [,global])
psb_normi(x, desc_a, info [,global])
```

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

Table 4: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 4.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

global Specifies whether the computation should include the global reduction across all processes.
Scope: **global**
Type: **optional**.
Intent: **in**.
Specified as: a logical scalar. Default: `global=.true.`

On Return

Function value is the infinity norm of vector x.
Scope: **global** unless the optional variable `global=.false.` has been specified
Specified as: a long precision real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. The computation of a global result requires a global communication, which entails a significant overhead. It may be necessary and/or advisable to compute multiple norms at the same time; in this case, it is possible to improve the runtime efficiency by using the following scheme:

```
vres(1) = psb_geamax(x1,desc_a,info,global=.false.)
vres(2) = psb_geamax(x2,desc_a,info,global=.false.)
vres(3) = psb_geamax(x3,desc_a,info,global=.false.)
call psb_amx(ctxt,vres(1:3))
```

   In this way the global communication, which for small sizes is a latency-bound operation, is invoked only once.

4.5 psb_geamaxs — Generalized Infinity Norm

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

$$res(i) \leftarrow \max_k |x(k,i)|$$

```
call psb_geamaxs(res, x, desc_a, info)
```

res	*x*	**Subroutine**
Short Precision Real	Short Precision Real	psb_geamaxs
Long Precision Real	Long Precision Real	psb_geamaxs
Short Precision Real	Short Precision Complex	psb_geamaxs
Long Precision Real	Long Precision Complex	psb_geamaxs

Table 5: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 5.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

On Return

res is the infinity norm of the columns of x.
Scope: **global**
Intent: **out**.
Specified as: a number or a rank-one array of long precision real numbers.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.6 psb_norm1 — 1-Norm of Vector

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

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

else if x is a complex vector then it computes 1-norm as:

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

`psb_geasum(x, desc_a, info [,global])` `psb_norm1(x, desc_a, info [,global])`

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

Table 6: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 6.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

global Specifies whether the computation should include the global reduction across all processes.
Scope: **global**
Type: **optional**.
Intent: **in**.
Specified as: a logical scalar. Default: `global=.true.`

On Return

Function value is the 1-norm of vector x.
Scope: **global** unless the optional variable `global=.false.` has been specified
Specified as: a long precision real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. The computation of a global result requires a global communication, which entails a significant overhead. It may be necessary and/or advisable to compute multiple norms at the same time; in this case, it is possible to improve the runtime efficiency by using the following scheme:

```
vres(1) = psb_geasum(x1,desc_a,info,global=.false.)
      vres(2) = psb_geasum(x2,desc_a,info,global=.false.)
      vres(3) = psb_geasum(x3,desc_a,info,global=.false.)
      call psb_sum(ctxt,vres(1:3))
```

   In this way the global communication, which for small sizes is a latency-bound operation, is invoked only once.

4.7 psb_geasums — Generalized 1-Norm of Vector

This subroutine computes a series of 1-norms on the columns of a dense matrix x:

$$res(i) \leftarrow \max_k |x(k,i)|$$

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

$$res(i) \leftarrow \|x_i\|$$

else if x is a complex vector then it computes 1-norm as:

$$res(i) \leftarrow \|re(x)\|_1 + \|im(x)\|_1$$

```
call psb_geasums(res, x, desc_a, info)
```

res	*x*	**Subroutine**
Short Precision Real	Short Precision Real	psb_geasums
Long Precision Real	Long Precision Real	psb_geasums
Short Precision Real	Short Precision Complex	psb_geasums
Long Precision Real	Long Precision Complex	psb_geasums

Table 7: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type containing numbers of type specified in Table 7.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_desc_type.

On Return

res contains the 1-norm of (the columns of) x.
Scope: **global**
Intent: **out**.
Short as: a long precision real number. Specified as: a long precision real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.8 psb_norm2 — 2-Norm of Vector

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

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

else if x is a complex vector then it computes 2-norm as:

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

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

Table 8: Data types

```
   psb_genrm2(x, desc_a, info [,global])
psb_norm2(x, desc_a, info [,global])
```

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 8.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

global Specifies whether the computation should include the global reduction across all processes.
Scope: **global**
Type: **optional**.
Intent: **in**.
Specified as: a logical scalar. Default: `global=.true.`

On Return

Function Value is the 2-norm of vector x.
Scope: **global** unless the optional variable `global=.false.` has been specified
Type: **required**
Specified as: a long precision real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. The computation of a global result requires a global communication, which entails a significant overhead. It may be necessary and/or advisable to compute multiple norms at the same time; in this case, it is possible to improve the runtime efficiency by using the following scheme:

```
vres(1) = psb_genrm2(x1,desc_a,info,global=.false.)
vres(2) = psb_genrm2(x2,desc_a,info,global=.false.)
vres(3) = psb_genrm2(x3,desc_a,info,global=.false.)
call psb_nrm2(ctxt,vres(1:3))
```

   In this way the global communication, which for small sizes is a latency-bound operation, is invoked only once.

4.9 psb_genrm2s — Generalized 2-Norm of Vector

This subroutine computes a series of 2-norms on the columns of a dense matrix x:

$$res(i) \leftarrow \|x(:,i)\|_2$$

```
call psb_genrm2s(res, x, desc_a, info)
```

res	*x*	**Subroutine**
Short Precision Real	Short Precision Real	psb_genrm2s
Long Precision Real	Long Precision Real	psb_genrm2s
Short Precision Real	Short Precision Complex	psb_genrm2s
Long Precision Real	Long Precision Complex	psb_genrm2s

Table 9: Data types

Type: Synchronous.

On Entry

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 9.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

On Return

res contains the 1-norm of (the columns of) x.
Scope: **global**
Intent: **out**.
Specified as: a long precision real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.10 psb_norm1 — 1-Norm of Sparse Matrix

This function computes the 1-norm of a matrix A:

$$nrm1 \leftarrow \|A\|_1$$

where:

A represents the global matrix A

A	**Function**
Short Precision Real	psb_spnrm1
Long Precision Real	psb_spnrm1
Short Precision Complex	psb_spnrm1
Long Precision Complex	psb_spnrm1

Table 10: Data types

```
psb_spnrm1(A, desc_a, info)
psb_norm1(A, desc_a, info)
```

Type: Synchronous.

On Entry

a the local portion of the global sparse matrix A.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_Tspmat_type.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_desc_type.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.11 psb_normi — 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**
Short Precision Real	psb_spnrmi
Long Precision Real	psb_spnrmi
Short Precision Complex	psb_spnrmi
Long Precision Complex	psb_spnrmi

Table 11: Data types

```
psb_spnrmi(A, desc_a, info)
psb_normi(A, desc_a, info)
```

Type: Synchronous.

On Entry

a the local portion of the global sparse matrix A.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_Tspmat_type.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object 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 Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.12 psb_spmm — Sparse Matrix by Dense Matrix Product

This subroutine computes the Sparse Matrix by Dense Matrix Product:

$$y \leftarrow \alpha Ax + \beta y \tag{1}$$

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

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

where:

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

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

A is the global sparse matrix A

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

Table 12: Data types

```
   call psb_spmm(alpha, a, x, beta, y, desc_a, info)
call psb_spmm(alpha, a, x, beta, y,desc_a, info, trans, work)
```

Type: Synchronous.

On Entry

alpha the scalar α.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 12.

a the local portion of the sparse matrix A.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_Tspmat_type.

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type containing numbers of type specified in Table 12. The rank of x must be the same of y.

beta the scalar β.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 12.

y the local portion of global dense matrix y.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 12. The rank of y must be the same of x.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

trans indicates 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**
Intent: **in**.
Default: $trans = N$
Specified as: a character variable.

work work array.
Scope: **local**
Type: **optional**
Intent: **inout**.
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 matrix y.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: an array of rank one or two containing numbers of type specified in Table 12.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.13 psb_spsm — Triangular System Solve

This subroutine computes the Triangular System Solve:

$$
\begin{aligned}
y &\leftarrow \alpha T^{-1}x + \beta y \\
y &\leftarrow \alpha DT^{-1}x + \beta y \\
y &\leftarrow \alpha T^{-1}Dx + \beta y \\
y &\leftarrow \alpha T^{-T}x + \beta y \\
y &\leftarrow \alpha DT^{-T}x + \beta y \\
y &\leftarrow \alpha T^{-T}Dx + \beta y \\
y &\leftarrow \alpha T^{-H}x + \beta y \\
y &\leftarrow \alpha DT^{-H}x + \beta y \\
y &\leftarrow \alpha T^{-H}Dx + \beta y
\end{aligned}
$$

where:

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

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

T is the global sparse block triangular submatrix T

D is the scaling diagonal matrix.

```
    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)
```

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

Table 13: Data types

Type: Synchronous.

On Entry

alpha the scalar α.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 13.

t the global portion of the sparse matrix T.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object type specified in § 3.

x the local portion of global dense matrix x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 13. The rank of x must be the same of y.

beta the scalar β.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a number of the data type indicated in Table 13.

y the local portion of global dense matrix y.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type `psb_T_vect_type` containing numbers of type specified in Table 13. The rank of y must be the same of x.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object 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**
Intent: **in**.
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**
Intent: **in**.
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**
Intent: **in**.
Default: `psb_avg_`
Specified as: an integer variable.

diag the diagonal scaling matrix.
Scope: **local**
Type: **optional**
Intent: **in**.
Default: $diag(1) = 1(noscaling)$
Specified as: a rank one array containing numbers of the type indicated in Table 13.

work a work array.
Scope: **local**
Type: **optional**
Intent: **inout**.
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**
Intent: **inout**.
Specified as: an array of rank one or two containing numbers of type specified in Table 13.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.14 psb_gemlt — Entrywise Product

This function computes the entrywise product between two vectors x and y

$$dot \leftarrow x(i)y(i).$$

```
psb_gemlt(x, y, desc_a, info)
```

dot, *x*, *y*	**Function**
Short Precision Real	psb_gemlt
Long Precision Real	psb_gemlt
Short Precision Complex	psb_gemlt
Long Precision Complex	psb_gemlt

Table 14: Data types

Type: Synchronous.

On Entry

x the local portion of global dense vector x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_T_vect_type containing numbers of type specified in Table 2.

y the local portion of global dense vector y.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_T_vect_type containing numbers of type specified in Table 2.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type psb_desc_type.

On Return

y the local portion of result submatrix y.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: an object of type psb_T_vect_type containing numbers of the type indicated in Table 14.

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

Intent: **out**.
An integer value; 0 means no error has been detected.

4.15 psb_gediv — Entrywise Division

This function computes the entrywise division between two vectors x and y

$$/ \leftarrow x(i)/y(i).$$

```
psb_gediv(x, y, desc_a, info, [flag)
```

$/, x, y$	**Function**
Short Precision Real	psb_gediv
Long Precision Real	psb_gediv
Short Precision Complex	psb_gediv
Long Precision Complex	psb_gediv

Table 15: Data types

Type: Synchronous.

On Entry

x the local portion of global dense vector x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_T_vect_type` containing numbers of type specified in Table 2.

y the local portion of global dense vector y.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_T_vect_type` containing numbers of type specified in Table 2.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

flag check if any of the $y(i) = 0$, and in case returns error halting the computation.
Scope: **local**
Type: **optional** Intent: **in**.
Specified as: the logical value `flag=.true.`

On Return

x the local portion of result submatrix x.
Scope: **local**
Type: **required**
Intent: **inout**.

Specified as: an object of type psb_T_vect_type containing numbers of the type indicated in Table 14.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

4.16 psb_geinv — Entrywise Inversion

This function computes the entrywise inverse of a vector x and puts it into y

$$/ \leftarrow 1/x(i).$$

```
psb_geinv(x, y, desc_a, info, [flag)
```

$/, x, y$	**Function**
Short Precision Real	psb_geinv
Long Precision Real	psb_geinv
Short Precision Complex	psb_geinv
Long Precision Complex	psb_geinv

Table 16: Data types

Type: Synchronous.

On Entry

x the local portion of global dense vector x.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_T_vect_type` containing numbers of type specified in Table 2.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an object of type `psb_desc_type`.

flag check if any of the $x(i) = 0$, and in case returns error halting the computation.
Scope: **local**
Type: **optional** Intent: **in**.
Specified as: the logical value `flag=.true.`

On Return

y the local portion of result submatrix x.
Scope: **local**
Type: **required**
Intent: **out**.
Specified as: an object of type `psb_T_vect_type` containing numbers of the type indicated in Table 16.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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.

5.1 psb_halo — Halo Data Communication

These subroutines gathers the values of the halo elements:

$$x \leftarrow x$$

where:

x is a global dense submatrix.

α, x	**Subroutine**
Integer	psb_halo
Short Precision Real	psb_halo
Long Precision Real	psb_halo
Short Precision Complex	psb_halo
Long Precision Complex	psb_halo

Table 17: Data types

```
call psb_halo(x, desc_a, info)
call psb_halo(x, desc_a, info, work, data)
```

Type: Synchronous.

On Entry

x global dense matrix x.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type psb_T_vect_type containing numbers of type specified in Table 17.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_desc_type.

work the work array.
Scope: **local**
Type: **optional**
Intent: **inout**.
Specified as: a rank one array of the same type of x.

data index list selector.
Scope: **global**
Type: **optional**
Specified as: an integer. Values:psb_comm_halo_,psb_comm_mov_, psb_comm_ext_, default: psb_comm_halo_. Chooses the index list on which to base the data exchange.

On Return

x global dense result matrix x.
Scope: **local**
Type: **required**
Intent: **inout**.
Returned as: a rank one or two array containing numbers of type specified in Table 17.

info the local portion of result submatrix y.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value that contains an error code.

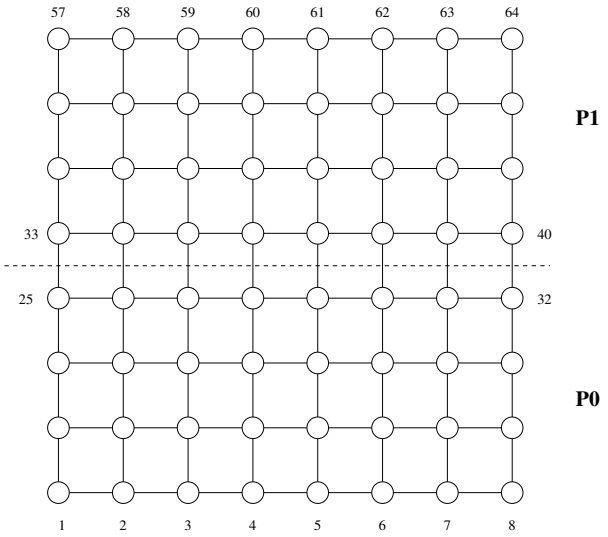

Figure 3: Sample discretization mesh.

Usage Example Consider the discretization mesh depicted in fig. 3, partitioned among two processes as shown by the dashed line; the data distribution is such that each process will own 32 entries in the index space, with a halo made of 8 entries placed at local indices 33 through 40. If process 0 assigns an initial value of 1 to its entries in the x vector, and process 1 assigns a value of 2, then after a call to `psb_halo` the contents of the local vectors will be the following:

	Process 0			Process 1	
I	GLOB(I)	X(I)	I	GLOB(I)	X(I)
1	1	1.0	1	33	2.0
2	2	1.0	2	34	2.0
3	3	1.0	3	35	2.0
4	4	1.0	4	36	2.0
5	5	1.0	5	37	2.0
6	6	1.0	6	38	2.0
7	7	1.0	7	39	2.0
8	8	1.0	8	40	2.0
9	9	1.0	9	41	2.0
10	10	1.0	10	42	2.0
11	11	1.0	11	43	2.0
12	12	1.0	12	44	2.0
13	13	1.0	13	45	2.0
14	14	1.0	14	46	2.0
15	15	1.0	15	47	2.0
16	16	1.0	16	48	2.0
17	17	1.0	17	49	2.0
18	18	1.0	18	50	2.0
19	19	1.0	19	51	2.0
20	20	1.0	20	52	2.0
21	21	1.0	21	53	2.0
22	22	1.0	22	54	2.0
23	23	1.0	23	55	2.0
24	24	1.0	24	56	2.0
25	25	1.0	25	57	2.0
26	26	1.0	26	58	2.0
27	27	1.0	27	59	2.0
28	28	1.0	28	60	2.0
29	29	1.0	29	61	2.0
30	30	1.0	30	62	2.0
31	31	1.0	31	63	2.0
32	32	1.0	32	64	2.0
33	33	2.0	33	25	1.0
34	34	2.0	34	26	1.0
35	35	2.0	35	27	1.0
36	36	2.0	36	28	1.0
37	37	2.0	37	29	1.0
38	38	2.0	38	30	1.0
39	39	2.0	39	31	1.0
40	40	2.0	40	32	1.0

5.2 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**
Short Precision Real	psb_ovrl
Long Precision Real	psb_ovrl
Short Precision Complex	psb_ovrl
Long Precision Complex	psb_ovrl

Table 18: Data types

```
call psb_ovrl(x, desc_a, info)
call psb_ovrl(x, desc_a, info, update=update_type, work=work)
```

Type: Synchronous.

On Entry

x global dense matrix x.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type psb_T_vect_type containing numbers of type specified in Table 18.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Default: $update\_type = psb\_avg\_$
Scope: **global**
Specified as: a integer variable.

work the work array.
Scope: **local**
Type: **optional**
Intent: **inout**.
Specified as: a one dimensional array of the same type of x.

On Return

x global dense result matrix x.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: an array of rank one or two containing numbers of type specified in Table 18.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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.

Example of use Consider the discretization mesh depicted in fig. 4, partitioned among two processes as shown by the dashed lines, with an overlap of 1 extra layer with respect to the partition of fig. 3; the data distribution is such that each process will own 40 entries in the index space, with an overlap of 16 entries placed at local indices 25 through 40; the halo will run from local index 41 through local index 48.. If process 0 assigns an initial value of 1 to its entries in the x vector, and process 1 assigns a value of 2, then after a call to `psb_ovrl` with `psb_avg_` and a call to `psb_halo_` the contents of the local vectors will be the following (showing a transition among the two subdomains)

	Process 0			Process 1	
I	GLOB(I)	X(I)	I	GLOB(I)	X(I)
1	1	1.0	1	33	1.5
2	2	1.0	2	34	1.5
3	3	1.0	3	35	1.5
4	4	1.0	4	36	1.5
5	5	1.0	5	37	1.5
6	6	1.0	6	38	1.5
7	7	1.0	7	39	1.5
8	8	1.0	8	40	1.5
9	9	1.0	9	41	2.0
10	10	1.0	10	42	2.0
11	11	1.0	11	43	2.0
12	12	1.0	12	44	2.0
13	13	1.0	13	45	2.0
14	14	1.0	14	46	2.0
15	15	1.0	15	47	2.0
16	16	1.0	16	48	2.0
17	17	1.0	17	49	2.0
18	18	1.0	18	50	2.0
19	19	1.0	19	51	2.0
20	20	1.0	20	52	2.0
21	21	1.0	21	53	2.0
22	22	1.0	22	54	2.0
23	23	1.0	23	55	2.0
24	24	1.0	24	56	2.0
25	25	1.5	25	57	2.0
26	26	1.5	26	58	2.0
27	27	1.5	27	59	2.0
28	28	1.5	28	60	2.0
29	29	1.5	29	61	2.0
30	30	1.5	30	62	2.0
31	31	1.5	31	63	2.0
32	32	1.5	32	64	2.0
33	33	1.5	33	25	1.5
34	34	1.5	34	26	1.5
35	35	1.5	35	27	1.5
36	36	1.5	36	28	1.5
37	37	1.5	37	29	1.5
38	38	1.5	38	30	1.5
39	39	1.5	39	31	1.5
40	40	1.5	40	32	1.5
41	41	2.0	41	17	1.0
42	42	2.0	42	18	1.0
43	43	2.0	43	19	1.0
44	44	2.0	44	20	1.0
45	45	2.0	45	21	1.0
46	46	2.0	46	22	1.0
47	47	2.0	47	23	1.0
48	48	2.0	48	24	1.0

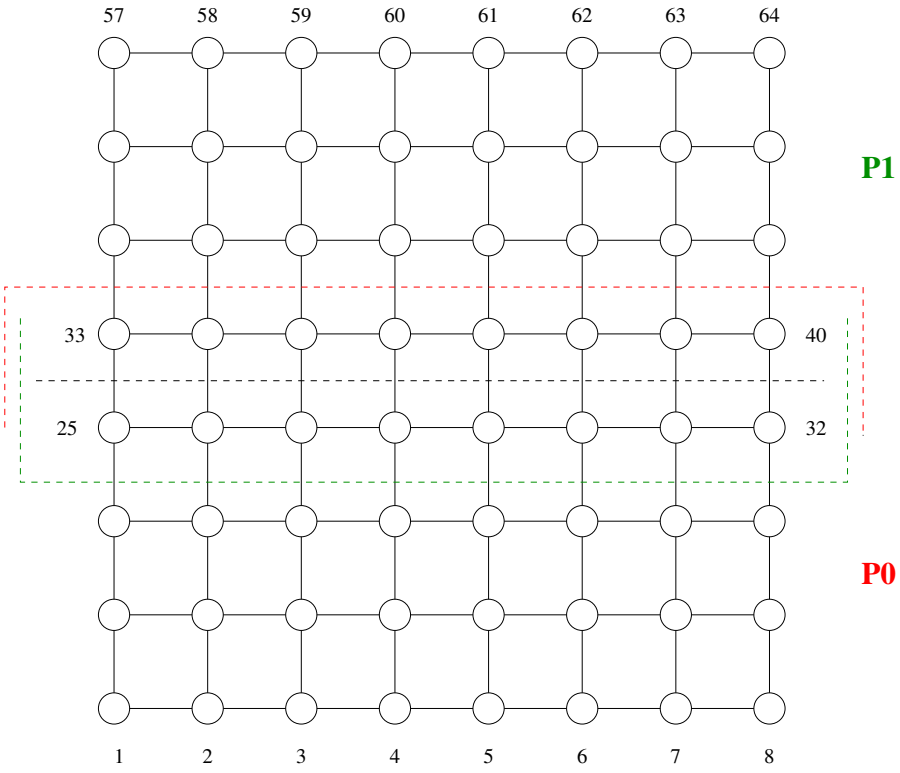

Figure 4: Sample discretization mesh.

5.3 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 $glob\_x_{1:m,1:n}$

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

$collect$ is the collect function.

x_i, y	**Subroutine**
Integer	psb_gather
Short Precision Real	psb_gather
Long Precision Real	psb_gather
Short Precision Complex	psb_gather
Long Precision Complex	psb_gather

Table 19: Data types

```
call psb_gather(glob_x, loc_x, desc_a, info, root) call psb_gather(glob_x, loc_x, desc
```

Type: Synchronous.

On Entry

loc_x the local portion of global dense matrix $glob\_x$.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array or an object of type psb_T_vect_type indicated in Table 19.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Specified as: an integer variable $-1 \leq root \leq np - 1$, default -1.

On Return

glob_x The array where the local parts must be gathered.
Scope: **global**
Type: **required**
Intent: **out**.
Specified as: a rank one or two array with the `ALLOCATABLE` attribute.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

5.4 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.

$$loc\_x_i \leftarrow scatter(glob\_x)$$

where:

$glob\_x$ is the global matrix $glob\_x_{1:m,1:n}$

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

$scatter$ is the scatter function.

x_i, y	**Subroutine**
Integer	psb_scatter
Short Precision Real	psb_scatter
Long Precision Real	psb_scatter
Short Precision Complex	psb_scatter
Long Precision Complex	psb_scatter

Table 20: Data types

```
call psb_scatter(glob_x, loc_x, desc_a, info, root, mold)
```

Type: Synchronous.

On Entry

glob_x The array that must be scattered into local pieces.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a rank one or two array.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Specified as: an integer variable $-1 \leq root \leq np - 1$, default psb_root_, i.e. process 0.

mold The desired dynamic type for the internal vector storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from `psb_T_base_vect_type`; this is only allowed when loc_x is of type `psb_T_vect_type`.

On Return

loc_x the local portion of global dense matrix *glob_x*.
Scope: **local**
Type: **required**
Intent: **out**.
Specified as: a rank one or two ALLOCATABLE array or an object of type `psb_T_vect_type` containing numbers of the type indicated in Table 20.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6 Data management routines

6.1 psb_cdall — Allocates a communication descriptor

```
call psb_cdall(icontxt, desc_a, info,mg=mg,parts=parts)
call psb_cdall(icontxt, desc_a, info,vg=vg,[mg=mg,flag=flag])
call psb_cdall(icontxt, desc_a, info,vl=vl,[nl=nl,globalcheck=.false.,lidx=lidx])
call psb_cdall(icontxt, desc_a, info,nl=nl)
call psb_cdall(icontxt, desc_a, info,mg=mg,repl=.true.)
```

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

On Entry

Type: Synchronous.

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

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

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

mg the (global) number of rows of the problem.
Scope:**global**.
Type:**optional**.
Intent: **in**.
Specified as: an integer value. It is required if `parts` or `repl` is specified, it is optional if `vg` 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 $vl(1 : nl)$ belonging to the calling process.
Scope:**local**.
Type:**optional**.
Intent: **in**.
Specified as: an integer array.

nl Data allocation: in a generalized block-row distribution the number of indices belonging to the current process.
Scope:**local**.
Type:**optional**.
Intent: **in**.
Specified as: an integer value. May be specified together with `vl`.

repl Data allocation: build a replicated index space (i.e. all processes own all indices).
Scope:**global**.
Type:**optional**.
Intent: **in**.
Specified as: the logical value `.true.`

globalcheck Data allocation: do global checks on the local index lists `vl`
Scope:**global**.
Type:**optional**.
Intent: **in**.
Specified as: a logical value, default: `.false.`

lidx Data allocation: the set of local indices $lidx(1:nl)$ to be assigned to the global indices vl.
Scope:**local**.
Type:**optional**.
Intent: **in**.
Specified as: an integer array.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. One of the optional arguments `parts`, `vg`, `vl`, `nl` or `repl` must be specified, thereby choosing the initialization strategy as follows:

   parts In this case we have a subroutine specifying the mapping between global indices and process/local index pairs. If this optional argument is specified, then it is mandatory to specify the argument `mg` as well. The subroutine must conform to the following interface:

   ```
   interface
      subroutine psb_parts(glob_index,mg,np,pv,nv)
   ```

```
      integer, intent (in)  :: glob_index,np,mg
      integer, intent (out) :: nv, pv(*)
    end subroutine psb_parts
  end interface
```

The input arguments are:

glob_index The global index to be mapped;

np The number of processes in the mapping;

mg The total number of global rows in the mapping;

The output arguments are:

nv The number of entries in `pv`;

pv A vector containing the indices of the processes to which the global index should be assigend; each entry must satisfy $0 \leq pv(i) < np$; if $nv > 1$ we have an index assigned to multiple processes, i.e. we have an overlap among the subdomains.

vg In this case the association between an index and a process is specified via an integer vector `vg(1:mg)`; each index $i \in \{1 \ldots mg\}$ is assigned to 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`. The size mg may be specified via the optional argument `mg`; the default is to use the entire vector `vg`, thus having `mg=size(vg)`.

vl In this case we are specifying the list of indices `vl(1:nl)` assigned to the current process; thus, the global problem size mg is given by the range of the aggregate of the individual vectors `vl` specified in the calling processes. The size may be specified via the optional argument `nl`; the default is to use the entire vector `vl`, thus having `nl=size(vl)`. If `globalcheck=.true.` the subroutine will check how many times each entry in the global index space $(1 \ldots mg)$ is specified in the input lists `vl`, thus allowing for the presence of overlap in the input, and checking for "orphan" indices. If `globalcheck=.false.`, the subroutine will not check for overlap, and may be significantly faster, but the user is implicitly guaranteeing that there are neither orphan nor overlap indices.

lidx The optional argument `lidx` is available for those cases in which the user has already established a global-to-local mapping; if it is specified, each index in `vl(i)` will be mapped to the corresponding local index `lidx(i)`. When specifying the argument `lidx` the user would also likely employ `lidx` in calls to `psb_cdins` and `local` in calls to `psb_spins` and `psb_geins`; see also sec. 2.3.1.

nl If this argument is specified alone (i.e. without `vl`) the result is a generalized row-block distribution in which each process I gets assigned a consecutive chunk of $N_I = nl$ global indices.

repl This arguments specifies to replicate all indices on all processes. This is a special purpose data allocation that is useful in the construction of some multilevel preconditioners.

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

3. Calling the routine with `vg` or `parts` implies that every process will scan the entire index space to figure out the local indices.

4. Overlapped indices are possible with both `parts` and `vl` invocations.

5. When the subroutine is invoked with `vl` in conjunction with `globalcheck=.true.`, it will perform a scan of the index space to search for overlap or orphan indices.

6. When the subroutine is invoked with `vl` in conjunction with `globalcheck=.false.`, no index space scan will take place. Thus it is the responsibility of the user to make sure that the indices specified in `vl` have neither orphans nor overlaps; if this assumption fails, results will be unpredictable.

7. Orphan and overlap indices are impossible by construction when the subroutine is invoked with `nl` (alone), or `vg`.

6.2 psb_cdins — Communication descriptor insert routine

```
call psb_cdins(nz, ia, ja, desc_a, info [,ila,jla])
call psb_cdins(nz,ja,desc,info[,jla,mask,lidx])
```

This subroutine examines the edges of the graph associated with the discretization mesh (and isomorphic to the sparsity pattern of a linear system coefficient matrix), storing them as necessary into the communication descriptor. In the first form the edges are specified as pairs of indices $ia(i), ja(i)$; the starting index $ia(i)$ should belong to the current process. In the second form only the remote indices $ja(i)$ are specified.

Type: Asynchronous.

On Entry

nz the number of points being inserted.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: an integer value.

ia the indices of the starting vertex of the edges being inserted.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: an integer array of length nz.

ja the indices of the end vertex of the edges being inserted.
Scope: **local**.
Type: **required**.
Intent: **in**.
Specified as: an integer array of length nz.

mask Mask entries in `ja`, they are inserted only when the corresponding `mask` entries are `.true.`
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: a logical array of length nz, default `.true.`.

lidx User defined local indices for `ja`.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an integer array of length nz.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

ila the local indices of the starting vertex of the edges being inserted.
Scope: **local**.
Type: **optional**.
Intent: **out**.
Specified as: an integer array of length *nz*.

jla the local indices of the end vertex of the edges being inserted.
Scope: **local**.
Type: **optional**.
Intent: **out**.
Specified as: an integer array of length *nz*.

Notes

1. This routine may only be called if the descriptor is in the build state;
2. This routine automatically ignores edges that do not insist on the current process, i.e. edges for which neither the starting nor the end vertex belong to the current process.
3. The second form of this routine will be useful when dealing with user-specified index mappings; see also 2.3.1.

6.3 psb_cdasb — Communication descriptor assembly routine

```
call psb_cdasb(desc_a, info [, mold])
```

Type: Synchronous.

On Entry

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

mold The desired dynamic type for the internal index storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: a object of type derived from (integer) psb_T_base_vect_type.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

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

This call will set up all the necessary information for the halo data exchanges. In doing so, the library will need to identify the set of processes owning the halo indices through the use of the desc%fnd_owner() method; the owning processes are the topological neighbours of the calling process. If the user has some background information on the processes that are neighbours of the current one, it is possible to specify explicitly the list of adjacent processes with a call to desc%set_p_adjcncy(list); this will speed up the subsequent call to psb_cdasb.

6.4 psb_cdcpy — Copies a communication descriptor

```
call psb_cdcpy(desc_in, desc_out, info)
```

Type: Asynchronous.

On Entry

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

On Return

desc_out the communication descriptor copy.
Scope:**local**.
Type:**required**.
Intent: **out**.
Specified as: a structured data of type psb_desc_type.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.5 psb_cdfree — Frees a communication descriptor

```
call psb_cdfree(desc_a, info)
```

Type: Synchronous.

On Entry

desc_a the communication descriptor to be freed.
Scope:**local**.
Type:**required**.
Intent: **inout**.
Specified as: a structured data of type psb_desc_type.

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.6 psb_cdbldext — Build an extended communication descriptor

```
call psb_cdbldext(a,desc_a,nl,desc_out, info, extype)
```

This subroutine builds an extended communication descriptor, based on the input descriptor `desc_a` and on the stencil specified through the input sparse matrix `a`.

Type: Synchronous.

On Entry

a A sparse matrix Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: a structured data type.

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

nl the number of additional layers desired.
Scope:**global**.
Type:**required**.
Intent: **in**.
Specified as: an integer value $nl \geq 0$.

extype the kind of estension required.
Scope:**global**.
Type:**optional** .
Intent: **in**.
Specified as: an integer value `psb_ovt_xhal_`, `psb_ovt_asov_`, default: `psb_ovt_xhal_`

On Return

desc_out the extended communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **inout**.
Specified as: a structured data of type `psb_desc_type`.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. Specifying `psb_ovt_xhal_` for the `extype` argument the user will obtain a descriptor for a domain partition in which the additional layers are fetched as part of an (extended) halo; however the index-to-process mapping is identical to that of the base descriptor;
2. Specifying `psb_ovt_asov_` for the `extype` argument the user will obtain a descriptor with an overlapped decomposition: the additional layer is aggregated to the local subdomain (and thus is an overlap), and a new halo extending beyond the last additional layer is formed.

6.7 psb_spall — Allocates a sparse matrix

```
call psb_spall(a, desc_a, info [, nnz, dupl, bldmode])
```

Type: Synchronous.

On Entry

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**.
Intent: **in**.
Specified as: an integer value.

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

bldmode Whether to keep track of matrix entries that do not belong to the current process.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value psb_matbld_noremote_, psb_matbld_remote_.
Default: psb_matbld_noremote_.

On Return

a the matrix to be allocated.
Scope:**local**
Type:**required**
Intent: **out**.
Specified as: a structured data of type psb_Tspmat_type.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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;

4. Using `psb_matbld_remote_` is likely to cause a runtime overhead at assembly time;

6.8 psb_spins — Insert a set of coefficients into a sparse matrix

```
call psb_spins(nz, ia, ja, val, a, desc_a, info [,local])
call psb_spins(nr, irw, irp, ja, val, a, desc_a, info [,local])
```

Type: Asynchronous.

On Entry

nz the number of coefficients to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer scalar.

nr the number of rows to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer scalar.

irw the first row to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer scalar.

ia the row indices of the coefficients to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer array of size nz.

irp the row pointers of the coefficients to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer array of size $nr + 1$.

ja the column indices of the coefficients to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an integer array of size nz.

val the coefficients to be inserted.
Scope:**local**.
Type:**required**.
Intent: **in**.
Specified as: an array of size nz. Must be of the same type and kind of the coefficients of the sparse matrix a.

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

local Whether the entries in the indices vectors ia, ja are already in local numbering.
Scope:**local**.
Type:**optional**.
Specified as: a logical value; default: .false..

On Return

a the matrix into which coefficients will be inserted.
Scope:**local**
Type:**required**
Intent: **inout**.
Specified as: a structured data of type psb_Tspmat_type.

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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 must also be in the build state; the action of the routine is to (implicitly) call psb_cdins to add entries to the sparsity pattern; each sparse matrix entry implicitly defines a graph edge, that is passed to the descriptor routine for the appropriate processing;

4. The input data can be passed in either COO or CSR formats;

5. In COO format the coefficients to be inserted are represented by the ordered triples $ia(i), ja(i), val(i)$, for $i = 1, \ldots, nz$; these triples are arbitrary;

6. In CSR format the coefficients to be inserted for each input row $i = 1, nr$ are represented by the ordered triples $(i + irw - 1), ja(j), val(j)$, for $j = irp(i), \ldots, irp(i+1) - 1$; these triples should belong to the current process, i.e. $i + irw - 1$ should be one of the local indices, but are otherwise arbitrary;

7. There is no requirement that a given row must be passed in its entirety to a single call to this routine: the buildup of a row may be split into as many calls as desired (even in the CSR format);

8. Coefficients from different rows may also be mixed up freely in a single call, according to the application needs;

9. Coefficients from matrix rows not owned by the calling process are treated according to the value of `bldmode` specified at allocation time; if `bldmode` was chosen as `psb_matbld_remote_` the library will keep track of them, otherwise they are silently ignored;

10. If the descriptor is in the assembled state, then any entries in the sparse matrix that would generate additional communication requirements are ignored;

11. If the matrix is in the update state, any entries in positions that were not present in the original matrix are ignored.

6.9 psb_spasb — Sparse matrix assembly routine

```
call psb_spasb(a, desc_a, info [, afmt, upd,  mold])
```

Type: Synchronous.

On Entry

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

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

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

mold The desired dynamic type for the internal matrix storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from psb_T_base_sparse_mat.

On Return

a the matrix to be assembled.
Scope:**local**
Type:**required**
Intent: **inout**.
Specified as: a structured data of type psb_Tspmat_type.

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in/out**.
Specified as: a structured data of type psb_desc_type. If the matrix was allocated with bldmode=psb_matbld_remote_, then the descriptor will be reassembled.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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. The output storage format need not be the same on all processes;
6. On exit from this routine the matrix is in the assembled state, and thus is suitable for the computational routines;
7. If the `bldmode=psb_matbld_remote_` value was specified at allocation time, contributions defined on the current process but belonging to a remote process will be handled accordingly. This is most likely to occur in finite element applications, with `dupl=psb_dupl_add_`; it is necessary to check for possible updates needed in the descriptor, hence there will be a runtime overhead.

6.10 psb_spfree — Frees a sparse matrix

```
call psb_spfree(a, desc_a, info)
```

Type: Synchronous.

On Entry

a the matrix to be freed.
Scope:**local**
Type:**required**
Intent: **inout**.
Specified as: a structured data of type psb_Tspmat_type.

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

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.11 psb_sprn — Reinit sparse matrix structure for psblas routines.

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

Type: Synchronous.

On Entry

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

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

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

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

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

6.12 psb_geall — Allocates a dense matrix

```
call psb_geall(x, desc_a, info[, dupl, bldmode, n, lb])
```

Type: Synchronous.

On Entry

desc_a The communication descriptor.
Scope: **local**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Specified as: Integer scalar, default 1. It is not a valid argument if x is a rank-1 array.

lb The lower bound for the column index range of the dense matrix to be allocated.
Scope: **local**
Type: **optional**
Intent: **in**.
Specified as: Integer scalar, default 1. It is not a valid argument if x is a rank-1 array.

dupl How to handle duplicate coefficients.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: integer, possible values: psb_dupl_ovwrt_, psb_dupl_add_; psb_dupl_err_ has no effect.

bldmode Whether to keep track of matrix entries that do not belong to the current process.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value psb_matbld_noremote_, psb_matbld_remote_.
Default: psb_matbld_noremote_.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. Using `psb_matbld_remote_` is likely to cause a runtime overhead at assembly time;

6.13 psb_geins — Dense matrix insertion routine

```
call psb_geins(m, irw, val, x, desc_a, info [,local])
```

Type: Asynchronous.

On Entry

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

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

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

local Whether the entries in the index vector `irw`, are already in local numbering.
Scope:**local**.
Type:**optional**.
Specified as: a logical value; default: `.false.`.

On Return

x the output dense matrix.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one or two array or an object of type psb_T_vect_type, of type real, complex or integer.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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.

6.14 psb_geasb — Assembly a dense matrix

```
call psb_geasb(x, desc_a, info, mold)
```

Type: Synchronous.

On Entry

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

mold The desired dynamic type for the internal vector storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from psb_T_base_vect_type; this is only allowed when x is of type psb_T_vect_type.

On Return

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

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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. If the bldmode=psb_matbld_remote_ value was specified at allocation time, contributions defined on the current process but belonging to a remote process will be handled accordingly. This is most likely to occur in finite element applications, with dupl=psb_dupl_add_.

6.15 psb_gefree — Frees a dense matrix

```
call psb_gefree(x, desc_a, info)
```

Type: Synchronous.

On Entry

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

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

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.16 psb_gelp — Applies a left permutation to a dense matrix

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

Type: Asynchronous.

On Entry

trans A character that specifies whether to permute A or A^T.
Scope: **local**
Type: **required**
Intent: **in**.
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**
Intent: **in**.
Specified as: an integer one-dimensional array.

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

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.17 psb_glob_to_loc — Global to local indices convertion

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

Type: Asynchronous.

On Entry

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

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **in**.
Specified as: a character variable Ignore, Warning or Abort, default Ignore.

owned Specfies valid range of input Scope: **global**
Type: **optional**
Intent: **in**.
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**
Intent: **inout**.
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**
Intent: **out**.
Specified as: a rank one integer array.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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.

6.18 psb_loc_to_glob — Local to global indices conversion

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

Type: Asynchronous.

On Entry

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

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **in**.
Specified as: a character variable Ignore, Warning or Abort, default Ignore.

On Return

x If y is not present, then x is overwritten with the translated integer indices.
Scope: **global**
Type: **required**
Intent: **inout**.
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**
Intent: **out**.
Specified as: a rank one integer array.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

6.19 psb_is_owned —

```
call psb_is_owned(x, desc_a)
```

Type: Asynchronous.

On Entry

x Integer index.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a scalar integer.

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

On Return

Function value A logical mask which is true if x is owned by the current process Scope: **local**
Type: **required**
Intent: **out**.

Notes

1. This routine returns a `.true.` value for an index that is strictly owned by the current process, excluding the halo indices

6.20 psb_owned_index —

```
call psb_owned_index(y, x, desc_a, info)
```

Type: Asynchronous.

On Entry

x Integer indices.
Scope: **local**
Type: **required**
Intent: **in, inout**.
Specified as: a scalar or a rank one integer array.

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **in**.
Specified as: a character variable Ignore, Warning or Abort, default Ignore.

On Return

y A logical mask which is true for all corresponding entries of x that are owned by the current process Scope: **local**
Type: **required**
Intent: **out**.
Specified as: a scalar or rank one logical array.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. This routine returns a .true. value for those indices that are strictly owned by the current process, excluding the halo indices

6.21 psb_is_local —

```
call psb_is_local(x, desc_a)
```

Type: Asynchronous.

On Entry

x Integer index.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a scalar integer.

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

On Return

Function value A logical mask which is true if x is local to the current process
Scope: **local**
Type: **required**
Intent: **out**.

Notes

1. This routine returns a `.true.` value for an index that is local to the current process, including the halo indices

6.22 psb_local_index —

```
call psb_local_index(y, x, desc_a, info)
```

Type: Asynchronous.

On Entry

x Integer indices.
Scope: **local**
Type: **required**
Intent: **in, inout**.
Specified as: a scalar or a rank one integer array.

desc_a the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **in**.
Specified as: a character variable Ignore, Warning or Abort, default Ignore.

On Return

y A logical mask which is true for all corresponding entries of x that are local to the current process Scope: **local**
Type: **required**
Intent: **out**.
Specified as: a scalar or rank one logical array.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. This routine returns a .true. value for those indices that are local to the current process, including the halo indices.

6.23 psb_get_boundary — Extract list of boundary elements

```
call psb_get_boundary(bndel, desc, info)
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **out**.
Specified as: a rank one array with the ALLOCATABLE attribute, of type integer.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

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 the "not allocated" state.
2. Otherwise the size of `bndel` will be exactly equal to the number of boundary elements.

6.24 psb_get_overlap — Extract list of overlap elements

```
call psb_get_overlap(ovrel, desc, info)
```

Type: Asynchronous.

On Entry

desc the communication descriptor.
Scope:**local**.
Type:**required**.
Intent: **in**.
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**
Intent: **out**.
Specified as: a rank one array with the ALLOCATABLE attribute, of type integer.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. If there are no overlap elements the output vector is set to the "not allocated" state.
2. Otherwise the size of `ovrel` will be exactly equal to the number of overlap elements.

6.25 psb_sp_getrow — Extract row(s) from a sparse matrix

```
call psb_sp_getrow(row, a, nz, ia, ja, val, info, &
             & append, nzin, lrw)
```

Type: Asynchronous.

On Entry

row The (first) row to be extracted.
Scope:**local**
Type:**required**
Intent: **in**.
Specified as: an integer > 0.

a the matrix from which to get rows.
Scope:**local**
Type:**required**
Intent: **in**.
Specified as: a structured data of type psb_Tspmat_type.

append Whether to append or overwrite existing output.
Scope:**local**
Type:**optional**
Intent: **in**.
Specified as: a logical value default: false (overwrite).

nzin Input size to be appended to.
Scope:**local**
Type:**optional**
Intent: **in**.
Specified as: an integer > 0. When append is true, specifies how many entries in the output vectors are already filled.

lrw The last row to be extracted.
Scope:**local**
Type:**optional**
Intent: **in**.
Specified as: an integer > 0, default: *row*.

On Return

nz the number of elements returned by this call.
Scope:**local**.
Type:**required**.
Intent: **out**.
Returned as: an integer scalar.

ia the row indices.
Scope:**local**.
Type:**required**.
Intent: **inout**.
Specified as: an integer array with the ALLOCATABLE attribute.

ja the column indices of the elements to be inserted.
Scope:**local**.
Type:**required**.
Intent: **inout**.
Specified as: an integer array with the `ALLOCATABLE` attribute.

val the elements to be inserted.
Scope:**local**.
Type:**required**.
Intent: **inout**.
Specified as: a real array with the `ALLOCATABLE` attribute.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes

1. The output nz is always the size of the output generated by the current call; thus, if `append=.true.`, the total output size will be $nzin + nz$, with the newly extracted coefficients stored in entries `nzin+1:nzin+nz` of the array arguments;

2. When `append=.true.` the output arrays are reallocated as necessary;

3. The row and column indices are returned in the local numbering scheme; if the global numbering is desired, the user may employ the `psb_loc_to_glob` routine on the output.

6.26 psb_sizeof — Memory occupation

This function computes the memory occupation of a PSBLAS object.

```
isz = psb_sizeof(a)
isz = psb_sizeof(desc_a)
isz = psb_sizeof(prec)
```

Type: Asynchronous.

On Entry

a A sparse matrix A.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_Tspmat_type.

desc_a Communication descriptor.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_desc_type.

prec Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a preconditioner data structure psb_Tprec_type.

On Return

Function value The memory occupation of the object specified in the calling sequence, in bytes.
Scope: **local**
Returned as: an integer(psb_long_int_k_) number.

6.27 Sorting utilities —

psb_msort — Sorting by the Merge-sort algorithm
psb_qsort — Sorting by the Quicksort algorithm
psb_hsort — Sorting by the Heapsort algorithm

```
call psb_msort(x,ix,dir,flag)
call psb_qsort(x,ix,dir,flag)
call psb_hsort(x,ix,dir,flag)
```

These serial routines sort a sequence X into ascending or descending order. The argument meaning is identical for the three calls; the only difference is the algorithm used to accomplish the task (see Usage Notes below).

Type: Asynchronous.

On Entry

x The sequence to be sorted.
Type:**required**.
Specified as: an integer, real or complex array of rank 1.

ix A vector of indices.
Type:**optional**.
Specified as: an integer array of (at least) the same size as X.

dir The desired ordering.
Type:**optional**.
Specified as: an integer value:

Integer and real data: `psb_sort_up_`, `psb_sort_down_`, `psb_asort_up_`, `psb_asort_down_`; default `psb_sort_up_`.

Complex data: `psb_lsort_up_`, `psb_lsort_down_`, `psb_asort_up_`, `psb_asort_down_`; default `psb_lsort_up_`.

flag Whether to keep the original values in IX.
Type:**optional**.
Specified as: an integer value `psb_sort_ovw_idx_` or `psb_sort_keep_idx_`; default `psb_sort_ovw_idx_`.

On Return

x The sequence of values, in the chosen ordering.
Type:**required**.
Specified as: an integer, real or complex array of rank 1.

ix A vector of indices.
Type: **Optional**
An integer array of rank 1, whose entries are moved to the same position as the corresponding entries in x.

Notes

1. For integer or real data the sorting can be performed in the up/down direction, on the natural or absolute values;
2. For complex data the sorting can be done in a lexicographic order (i.e.: sort on the real part with ties broken according to the imaginary part) or on the absolute values;
3. The routines return the items in the chosen ordering; the output difference is the handling of ties (i.e. items with an equal value) in the original input. With the merge-sort algorithm ties are preserved in the same relative order as they had in the original sequence, while this is not guaranteed for quicksort or heapsort;
4. If $flag = psb\_sort\_ovw\_idx\_$ then the entries in $ix(1:n)$ where n is the size of x are initialized to $ix(i) \leftarrow i$; thus, upon return from the subroutine, for each index i we have in $ix(i)$ the position that the item $x(i)$ occupied in the original data sequence;
5. If $flag = psb\_sort\_keep\_idx\_$ the routine will assume that the entries in $ix(:)$ have already been initialized by the user;
6. The three sorting algorithms have a similar $O(n \log n)$ expected running time; in the average case quicksort will be the fastest and merge-sort the slowest. However note that:
   (a) The worst case running time for quicksort is $O(n^2)$; the algorithm implemented here follows the well-known median-of-three heuristics, but the worst case may still apply;
   (b) The worst case running time for merge-sort and heap-sort is $O(n \log n)$ as the average case;
   (c) The merge-sort algorithm is implemented to take advantage of subsequences that may be already in the desired ordering prior to the subroutine call; this situation is relatively common when dealing with groups of indices of sparse matrix entries, thus merge-sort is the preferred choice when a sorting is needed by other routines in the library.

7 Parallel environment routines

7.1 psb_init — Initializes PSBLAS parallel environment

```
call psb_init(ctxt, np, basectxt, ids)
```

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

Type: Synchronous.

On Entry

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

basectxt the initial communication context. The new context will be defined from the processes participating in the initial one.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. Default: use MPI_COMM_WORLD.

ids Identities of the processes to use for the new context; the argument is ignored when `np` is not specified. This allows the processes in the new environment to be in an order different from the original one.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer array. Default: use the indices $(0 \ldots np-1)$.

On Return

ctxt the communication context identifying the virtual parallel machine, type `psb_ctxt_type`. Note that this is always a duplicate of `basectxt`, so that library communications are completely separated from other communication operations.
Scope: **global**.
Type: **required**.
Intent: **out**.
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 base parallel environment.

7.2 psb_info — Return information about PSBLAS parallel environment

```
call psb_info(ctxt, iam, np)
```

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

Type: Asynchronous.

On Entry

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

On Return

iam Identifier of current process in the PSBLAS virtual parallel machine.
Scope: **local**.
Type: **required**.
Intent: **out**.
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**.
Intent: **out**.
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 `ctxt` that any such process may execute is to `psb_exit`.

7.3 psb_exit — Exit from PSBLAS parallel environment

```
call psb_exit(ctxt)
call psb_exit(ctxt,close)
```

This subroutine exits from the PSBLAS parallel virtual machine.

Type: Synchronous.

On Entry

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

close Whether to close all data structures related to the virtual parallel machine, besides those associated with ctxt.
Scope: **global**.
Type: **optional**.
Intent: **in**.
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 `ctxt` in this situation.

2. A call to this routine with `close=.true.` implies a call to `MPI_Finalize`, after which no parallel routine may be called.

3. If the user whishes to use multiple communication contexts in the same program, or to enter and exit multiple times into the parallel environment, this routine may be called 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.

7.4 psb_get_mpi_comm — Get the MPI communicator

```
icomm = psb_get_mpi_comm(ctxt)
```

This function returns the MPI communicator associated with a PSBLAS context

Type: Asynchronous.

On Entry

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

On Return

Function value The MPI communicator associated with the PSBLAS virtual parallel machine.
Scope: **global**.
Type: **required**.
Intent: **out**.

Notes The subroutine version `psb_get_mpicomm` is still available but is deprecated.

7.5 psb_get_mpi_rank — Get the MPI rank

```
rank = psb_get_mpi_rank(ctxt, id)
```

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

Type: Asynchronous.

On Entry

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

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

On Return

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

Notes The subroutine version `psb_get_rank` is still available but is deprecated.

7.6 psb_wtime — Wall clock timing

```
time = psb_wtime()
```

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

Type: Asynchronous.

On Exit

Function value the elapsed time in seconds.
Returned as: a `real(psb_dpk_)` variable.

7.7 psb_barrier — Sinchronization point parallel environment

```
call psb_barrier(ctxt)
```

This subroutine acts as an explicit synchronization point for the PSBLAS parallel virtual machine.

Type: Synchronous.

On Entry

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

7.8 psb_abort — Abort a computation

```
call psb_abort(ctxt)
```

This subroutine aborts computation on the parallel virtual machine.

Type: Asynchronous.

On Entry

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

7.9 psb_bcast — Broadcast data

```
call psb_bcast(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

dat On the root process, the data to be broadcast.
Scope: **global**.
Type: **required**.
Intent: **inout**.
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 variable, which may be a scalar or rank 1 array. Type, kind, rank and size must agree on all processes.

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On all processes other than root, the broadcasted data.
Scope: **global**.

Type: **required**.
Intent: **inout**.
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, kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
call psb_bcast(ctxt,dat,&
     & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_bcast(ctxt,dat,mode=psb_collective_start_,&
     & request=bcast_request)
....... ! Do not access dat
call psb_bcast(ctxt,dat,mode=psb_collective_end_,&
     & request=bcast_request)
```

7.10 psb_sum — Global sum

```
call psb_sum(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

dat The local contribution to the global sum.
Scope: **global**.
Type: **required**.
Intent: **inout**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, kind, 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**.
Intent: **in**.
Specified as: an integer value $-1 <= root <= np - 1$, default -1.

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On destination process(es), the result of the sum operation.
Scope: **global**.
Type: **required**.

Intent: **inout**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array.
Type, kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
call psb_sum(ctxt,dat,&
     & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_sum(ctxt,dat,mode=psb_collective_start_,&
     & request=sum_request)
....... ! Do not access dat
call psb_sum(ctxt,dat,mode=psb_collective_end_,&
     & request=sum_request)
```

7.11 psb_max — Global maximum

```
call psb_max(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

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

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

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

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
call psb_max(ctxt,dat,&
     & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_max(ctxt,dat,mode=psb_collective_start_,&
     & request=max_request)
....... ! Do not access dat
call psb_max(ctxt,dat,mode=psb_collective_end_,&
     & request=max_request)
```

7.12 psb_min — Global minimum

```
call psb_min(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

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

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On destination process(es), the result of the minimum operation.
Scope: **global**.

Type: **required**.
Intent: **inout**.
Specified as: an integer or real variable, which may be a scalar, or a rank 1 or 2 array.
Type, kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
call psb_min(ctxt,dat,&
     & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_min(ctxt,dat,mode=psb_collective_start_,&
     & request=min_request)
....... ! Do not access dat
call psb_min(ctxt,dat,mode=psb_collective_end_,&
     & request=min_request)
```

7.13 psb_amx — Global maximum absolute value

```
call psb_amx(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

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

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On destination process(es), the result of the maximum operation.
Scope: **global**.

Type: **required**.
Intent: **inout**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array. Type, kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
  call psb_amx(ctxt,dat,&
       & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_amx(ctxt,dat,mode=psb_collective_start_,&
     & request=amx_request)
  ....... ! Do not access dat
  call psb_amx(ctxt,dat,mode=psb_collective_end_,&
       & request=amx_request)
```

7.14 psb_amn — Global minimum absolute value

```
call psb_amn(ctxt, dat [, root, mode, request])
```

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

Type: Synchronous.

On Entry

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

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

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On destination process(es), the result of the minimum operation.
Scope: **global**.

Type: **required**.
Intent: **inout**.
Specified as: an integer, real or complex variable, which may be a scalar, or a rank 1 or 2 array.
Type, kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

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.

2. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
call psb_amn(ctxt,dat,&
     & mode=ior(psb_collective_start_,psb_collective_end_))
```

3. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_amn(ctxt,dat,mode=psb_collective_start_,&
     & request=amn_request)
....... ! Do not access dat
call psb_amn(ctxt,dat,mode=psb_collective_end_,&
     & request=amn_request)
```

7.15 psb_nrm2 — Global 2-norm reduction

```
call psb_nrm2(ctxt, dat [, root, mode, request])
```

This subroutine implements a 2-norm value reduction operation based on the underlying communication library.

Type: Synchronous.

On Entry

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

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

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

mode Whether the call is started in non-blocking mode and completed later, or is executed synchronously.
Scope: **global**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. The action to be taken is determined by its bit fields, which can be set with bitwise `OR`. Basic action values are `psb_collective_start_`, `psb_collective_end_`. Default: both fields are selected (i.e. require synchronous completion).

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

On Return

dat On destination process(es), the result of the 2-norm reduction.
Scope: **global**.

Type: **required**.
Intent: **inout**.
Specified as: a real variable, which may be a scalar, or a rank 1 array.
Kind, rank and size must agree on all processes.

request A request variable to check for operation completion.
Scope: **local**.
Type: **optional**.
Intent: **inout**.
If `mode` does not specify synchronous completion, then this variable must be present.

Notes

1. This reduction is appropriate to compute the results of multiple (local) NRM2 operations at the same time.

2. Denoting by dat_i the value of the variable dat on process i, the output res is equivalent to the computation of

$$res = \sqrt{\sum_i dat_i^2},$$

with care taken to avoid unnecessary overflow.

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

4. The `mode` argument can be built with the bitwise `IOR()` operator; in the following example, the argument is forcing immediate completion, hence the `request` argument needs not be specified:

```
  call psb_nrm2(ctxt,dat,&
       & mode=ior(psb_collective_start_,psb_collective_end_))
```

5. When splitting the operation in two calls, the `dat` argument *must not* be accessed between calls:

```
call psb_nrm2(ctxt,dat,mode=psb_collective_start_,&
     & request=nrm2_request)
  ....... ! Do not access dat
  call psb_nrm2(ctxt,dat,mode=psb_collective_end_,&
       & request=nrm2_request)
```

7.16 psb_snd — Send data

```
call psb_snd(ctxt, dat, dst, m)
```

This subroutine sends a packet of data to a destination.

Type: Synchronous: see usage notes.

On Entry

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

dat The data to be sent.
Scope: **local**.
Type: **required**.
Intent: **in**.
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, kind 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**.
Intent: **in**.
Specified as: an integer value $0 <= dst <= np - 1$.

m Number of rows.
Scope: **global**.
Type: **Optional**.
Intent: **in**.
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

Notes

1. This subroutine implies a synchronization, but only between the calling process and the destination process dst.

7.17 psb_rcv — Receive data

```
call psb_rcv(ctxt, dat, src, m)
```

This subroutine receives a packet of data to a destination.

Type: Synchronous: see usage notes.

On Entry

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

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

m Number of rows.
Scope: **global**.
Type: **Optional**.
Intent: **in**.
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**.
Intent: **inout**.
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, kind and rank must agree on sender and receiver process; if *m* is not specified, size must agree as well.

Notes

1. This subroutine implies a synchronization, but only between the calling process and the source process *src*.

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, an error is detected, this variable is set to a value corresponding to a specific error code. Then this error code is also pushed on the error stack and then either control is returned to the caller routine or the execution is aborted, depending on the users choice. At the time when the execution is aborted, an error message is printed on standard output with a level of verbosity than can be chosen by the user. If the execution is not aborted, then, the caller routine checks the value returned in the `info` variable and, if not zero, an error condition is raised. This process continues on all the levels of nested calls until the level where the user decides to abort the program execution.

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

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

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

end subroutine psb_foo
```

Listing 5: 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...
```

Listing 6: A sample PSBLAS-3.0 error message. Process 0 detected an error condition inside the psb_cest subroutine

8.1 psb_errpush — Pushes an error code onto the error stack

```
call psb_errpush(err_c, r_name, i_err, a_err)
```

Type: Asynchronous.

On Entry

err_c the error code
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: an integer.

r_name the soutine where the error has been caught.
Scope: **local**
Type: **required**
Intent: **in**.
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.

8.2 psb_error — Prints the error stack content and aborts execution

```
call psb_error(icontxt)
```

Type: Asynchronous.

On Entry

icontxt the communication context.
Scope: **global**
Type: **optional**
Intent: **in**.
Specified as: an integer.

8.3 psb_set_errverbosity — Sets the verbosity of error messages

```
call psb_set_errverbosity(v)
```

Type: Asynchronous.

On Entry

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

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

```
call psb_set_erraction(err_act)
```

Type: Asynchronous.

On Entry

err_act the type of action.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: an integer. Possible values: `psb_act_ret`, `psb_act_abort`.

9 Utilities

We have some utilities available for input and output of sparse matrices; the interfaces to these routines are available in the module `psb_util_mod`.

9.1 hb_read — Read a sparse matrix from a file in the Harwell–Boeing format

```
call hb_read(a, iret, iunit, filename, b, mtitle)
```

Type: Asynchronous.

On Entry

filename The name of the file to be read.
Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default input unit 5 (i.e. standard input in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

On Return

a the sparse matrix read from file.
Type:**required**.
Specified as: a structured data of type psb_Tspmat_type.

b Rigth hand side(s).
Type: **Optional**
An array of type real or complex, rank 2 and having the ALLOCATABLE attribute; will be allocated and filled in if the input file contains a right hand side, otherwise will be left in the UNALLOCATED state.

mtitle Matrix title.
Type: **Optional**
A charachter variable of length 72 holding a copy of the matrix title as specified by the Harwell-Boeing format and contained in the input file.

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

9.2 hb_write — Write a sparse matrix to a file in the Harwell–Boeing format

```
call hb_write(a, iret, iunit, filename, key, rhs, mtitle)
```

Type: Asynchronous.

On Entry

a the sparse matrix to be written.
Type:**required**.
Specified as: a structured data of type psb_Tspmat_type.

b Rigth hand side.
Type: **Optional**
An array of type real or complex, rank 1 and having the ALLOCATABLE attribute; will be allocated and filled in if the input file contains a right hand side.

filename The name of the file to be written to.
Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default output unit 6 (i.e. standard output in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

key Matrix key.
Type: **Optional**
A charachter variable of length 8 holding the matrix key as specified by the Harwell-Boeing format and to be written to file.

mtitle Matrix title.
Type: **Optional**
A charachter variable of length 72 holding the matrix title as specified by the Harwell-Boeing format and to be written to file.

On Return

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

9.3 mm_mat_read — Read a sparse matrix from a file in the MatrixMarket format

```
call mm_mat_read(a, iret, iunit, filename)
```

Type: Asynchronous.

On Entry

filename The name of the file to be read.
Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default input unit 5 (i.e. standard input in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

On Return

a the sparse matrix read from file.
Type:**required**.
Specified as: a structured data of type psb_Tspmat_type.

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

9.4 mm_array_read — Read a dense array from a file in the MatrixMarket format

```
call mm_array_read(b, iret, iunit, filename)
```

Type: Asynchronous.

On Entry

filename The name of the file to be read.
Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default input unit 5 (i.e. standard input in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

On Return

b Rigth hand side(s).
Type: **required**
An array of type real or complex, rank 1 or 2 and having the ALLOCATABLE attribute, or an object of type psb_T_vect_type, of type real or complex.
Will be allocated and filled in if the input file contains a right hand side, otherwise will be left in the UNALLOCATED state.

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

9.5 mm_mat_write — Write a sparse matrix to a file in the MatrixMarket format

```
call mm_mat_write(a, mtitle, iret, iunit, filename)
```

Type: Asynchronous.

On Entry

a the sparse matrix to be written.
Type:**required**.
Specified as: a structured data of type psb_Tspmat_type.

mtitle Matrix title.
Type: **required**
A charachter variable holding a descriptive title for the matrix to be written to file.

filename The name of the file to be written to.
Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default output unit 6 (i.e. standard output in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

On Return

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

Notes

If this function is called on a matrix a on a distributed communicator only the local part is written in output. To get a single MatrixMarket file with the whole matrix when appropriate, e.g. for debugging purposes, one could *gather* the whole matrix on a single rank and then write it. Consider the following example for a *double* precision matrix

```
type(psb_ldspmat_type) :: aglobal

call psb_gather(aglobal,a,desc_a,info)
if (iam == psb_root_) then
        call mm_mat_write(aglobal,mtitle,info,filename)
end if
call psb_spfree(aglobal, desc_a, info)
```

To simplify this procedure in C, there is a utility function

```
psb_i_t psb_c_<s,d,c,z>global_mat_write(ah,cdh);
```

that produces exactly this result.

9.6 mm_array_write — Write a dense array from a file in the MatrixMarket format

```
call mm_array_write(b, vtitle, iret, iunit, filename)
```

Type: Asynchronous.

On Entry

b Rigth hand side(s).
Type: **required**
An array of type real or complex, rank 1 or 2, or an object of type psb_T_vect_type, of type real or complex; its contents will be written to disk.

filename The name of the file to be written.

vtitle Matrix title.
Type: **required**
A charachter variable holding a descriptive title for the vector to be written to file. Type:**optional**.
Specified as: a character variable containing a valid file name, or -, in which case the default input unit 5 (i.e. standard input in Unix jargon) is used. Default: -.

iunit The Fortran file unit number.
Type:**optional**.
Specified as: an integer value. Only meaningful if filename is not -.

On Return

iret Error code.
Type: **required**
An integer value; 0 means no error has been detected.

Notes

If this function is called on a vector v on a distributed communicator only the local part is written in output. To get a single MatrixMarket file with the whole vector when appropriate, e.g. for debugging purposes, one could *gather* the whole vector on a single rank and then write it. Consider the following example for a *double* precision vector

```
real(psb_dpk_), allocatable :: vglobal(:)

call psb_gather(vglobal,v,desc,info)
if (iam == psb_root_) then
call mm_array_write(vglobal,vtitle,info,filename)
end if
call deallocate(vglobal, stat=info)
```

To simplify this procedure in C, there is a utility function

```
psb_i_t psb_c_<s,d,c,z>global_vec_write(vh,cdh);
```

that produces exactly this result.

10 Preconditioner routines

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

- Diagonal Scaling
- Block Jacobi with ILU(0) factorization
- Block Jacobi with an approximate inverse

The supporting data type and subroutine interfaces are defined in the module `psb_prec_mod`. The old interfaces `psb_precinit` and `psb_precbld` are still supported for backward compatibility

10.1 init — Initialize a preconditioner

```
call prec%init(icontxt,ptype, info)
```

Type: Asynchronous.

On Entry

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

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

On Exit

prec Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure `psb_Tprec_type`.

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

Notes Legal inputs to this subroutine are interpreted depending on the *ptype* string as follows[4]:

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;

BJAC Precondition by a factorization or an approximante inverse of the block-diagonal of matrix A, where block boundaries are determined by the data allocation boundaries for each process; requires no communication. See also Table-21.

[4]The string is case-insensitive

10.2 Set — set preconditioner parameters

```
call p%set(what,val,info)
```

This method sets the parameters defining the subdomain solver when the preconditioner type is `BJAC`. More precisely, the parameter identified by `what` is assigned the value contained in `val`.

Arguments

`what` — `character(len=*)`.
The parameter to be set. It can be specified through its name; the string is case-insensitive. See Table 21.

`val` — `integer` *or* `character(len=*)` *or* `real(psb_spk_)` *or* `real(psb_dpk_)`, `intent(in)`.
The value of the parameter to be set. The list of allowed values and the corresponding data types is given in Table 21. When the value is of type `character(len=*)`, it is also treated as case insensitive.

`info` — `integer, intent(out)`.
Error code. If no error, 0 is returned. See Section 8 for details.

A number of subdomain solvers can be chosen with this method; a list of the parameters that can be set, along with their allowed and default values, is given in Table-21.

what	DATA TYPE	val	DEFAULT	COMMENTS
'SUB_SOLVE'	character(len=*)	'ILU' 'ILUT' 'INVT' 'INVK' 'AINV'		The local solver to be used with the smoother or one-level preconditioner ILU(p), ILU(p,t), Approximate Inverses INVK(p,q), INVT($p_1, p2, t_1, t_2$) and AINV(t); note that approximate inverses are specifically suited for GPUs since they do not employ triangular system solve kernels, see [2].
'SUB_FILLIN'	integer	Any integer number ≥ 0	0	Fill-in level p of the incomplete LU factorizations.
'SUB_ILUTHRS'	real(kind_parameter)	Any real number ≥ 0	0	Drop tolerance t in the ILU(p,t) factorization.
'ILU_ALG'	character(len=*)	'MILU'	'NONE'	ILU algorithmic variant
'ILUT_SCALE'	character(len=*)	'MAXVAL' 'DIAG' 'ARSWUM' 'ARCSUM' 'ACLSUM' 'NONE'	'NONE'	ILU scaling strategy
'INV_FILLIN'	integer	Any integer number ≥ 0	0	Second fill-in level q of the INVK(p,q) approximate inverse.
'INV_ILUTHRS'	real(kind_parameter)	Any real number ≥ 0	0	Second drop tolerance s in the INVT(t,s) approximate inverse.
'AINV_ALG'	character(len=*)	'LLK' 'SYM-LLK' 'STAB-LLK' 'MLK,LMX'	'LLK'	AINV algorithmic strategy.

Table 21: Parameters defining the solver of the BJAC preconditioner.

10.3 build — Builds a preconditioner

```
call prec%build(a, desc_a, info[,amold,vmold,imold])
```

Type: Synchronous.

On Entry

a the system sparse matrix. Scope: **local**
Type: **required**
Intent: **in**, target.
Specified as: a sparse matrix data structure psb_Tspmat_type.

prec the preconditioner.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: an already initialized precondtioner data structure psb_Tprec_type

desc_a the problem communication descriptor. Scope: **local**
Type: **required**
Intent: **in**, target.
Specified as: a communication descriptor data structure psb_desc_type.

amold The desired dynamic type for the internal matrix storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from psb_T_base_sparse_mat.

vmold The desired dynamic type for the internal vector storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from psb_T_base_vect_type.

imold The desired dynamic type for the internal integer vector storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from (integer) psb_T_base_vect_type.

On Return

prec the preconditioner.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a precondtioner data structure psb_Tprec_type

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

The `amold`, `vmold` and `imold` arguments may be employed to interface with special devices, such as GPUs and other accelerators.

10.4 apply — Preconditioner application routine

```
call prec%apply(x,y,desc_a,info,trans,work)
call prec%apply(x,desc_a,info,trans)
```

Type: Synchronous.

On Entry

prec the preconditioner. Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a preconditioner data structure psb_Tprec_type.

x the source vector. Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type psb_T_vect_type.

desc_a the problem communication descriptor. Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a communication data structure psb_desc_type.

trans Scope:
Type: **optional**
Intent: **in**.
Specified as: a character.

work an optional work space Scope: **local**
Type: **optional**
Intent: **inout**.
Specified as: a double precision array.

On Return

y the destination vector. Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type psb_T_vect_type.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

Notes This method is almost always called by the iterative methods of Sec. 11, and practically never directly by the user.

10.5 descr — Prints a description of current preconditioner

```
call prec%descr(info)
call prec%descr(info,iout, root)
```

Type: Asynchronous.

On Entry

prec the preconditioner. Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a preconditioner data structure psb_Tprec_type.

iout output unit. Scope: **local**
Type: **optional**
Intent: **in**.
Specified as: an integer number. Default: default output unit.

root Process from which to print Scope: **local**
Type: **optional**
Intent: **in**.
Specified as: an integer number between 0 and $np - 1$, in which case the specified process will print the description, or -1, in which case all processes will print. Default: 0.

On Return

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

10.6 clone — clone current preconditioner

```
call  prec%clone(precout,info)
```

Type: Asynchronous.

On Entry

prec the preconditioner.
Scope: **local**.

On Return

precout A copy of the input object.

info Return code.

10.7 free — Free a preconditioner

```
call prec%free(info)
```

Type: Asynchronous.

On Entry

prec the preconditioner.
Scope: **local**.
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

On Exit

prec Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

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

Notes Releases all internal storage.

10.8 allocate_wrk — preconditioner

```
call prec%allocate_wrk(info[,vmold])
```

Type: Synchronous.

On Entry

prec the preconditioner.
Scope: **local**.
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

vmold The desired dynamic type for the internal vector storage.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an object of a class derived from psb_T_base_vect_type.

On Exit

prec Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

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

Notes Preconditioners often need internal work storage during their application at each iteration of a linear solver method: in many situations this can be accomplished by allocating and releasing memory "on the fly". However, when running on an accelerator through e.g. the CUDA enabled data strutures of Sec. 12.4 and 13, memory allocation and deallocation usually have a much larger overhead, significantly affecting performance. To alleviate this problem we define this method that preallocates internal storage; it is intended to be invoked prior to the iterative solver method, so that the necessary internal scratch storage is available throughout the iterative method application.

When using GPUs or other specialized devices, the vmold argument is also necessary to ensure the internal work vectors are of the appropriate dynamic type to exploit the accelerator hardware.

10.9 deallocate_wrk — preconditioner

```
call prec%allocate_wrk(info)
call prec%free_wrk(info)
```

Type: Synchronous.

On Entry

prec the preconditioner.
Scope: **local**.
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

On Exit

prec Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a preconditioner data structure psb_Tprec_type.

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

Notes Deallocates preconditioner internal work storage; to be invoked after an iterative solver has completed execution, see the discussion in Sec. 10.8.

11 Iterative Methods

In this chapter we provide routines for preconditioners and iterative methods. The interfaces for iterative methods are available in the module `psb_linsolve_mod`.

11.1 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 version 2.

The stopping criterion can take the following values:

1 normwise backward error in the infinity norm; the iteration is stopped when

$$err = \frac{\|r_i\|}{(\|A\|\|x_i\| + \|b\|)} < eps$$

2 Relative residual in the 2-norm; the iteration is stopped when

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

3 Relative residual reduction in the 2-norm; the iteration is stopped when

$$err = \frac{\|r_i\|}{\|r_0\|_2} < eps$$

The behaviour is controlled by the istop argument (see later). In the above formulae, x_i is the tentative solution and $r_i = b - Ax_i$ the corresponding residual at the i-th iteration.

```
call psb_krylov(method,a,prec,b,x,eps,desc_a,info,&
     & itmax,iter,err,itrace,irst,istop,cond)
```

Type: Synchronous.

On Entry

method a string that defines the iterative method to be used. Supported values are:

- **CG:** the Conjugate Gradient method;
- **CGS:** the Conjugate Gradient Stabilized method;
- **GCR:** the Generalized Conjugate Residual method;
- **FCG:** the Flexible Conjugate Gradient method[5];
- **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**
Intent: **in**.
Specified as: a structured data of type psb_Tspmat_type.

[5]Note: the implementation is for $FCG(1)$.

prec The data structure containing the preconditioner.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_Tprec_type.

b The RHS vector.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one array or an object of type psb_T_vect_type.

x The initial guess.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type psb_T_vect_type.

eps The stopping tolerance.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a real number.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.
Scope: **global**
Type: **optional**
Intent: **in**.
Default: $itmax = 1000$.
Specified as: an integer variable $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every *itrace* iterations. If $= 0$ print a message in case of convergence failure.
Scope: **global**
Type: **optional**
Intent: **in**.
Default: $itrace = -1$.

irst An integer specifying the restart parameter.
Scope: **global**
Type: **optional**.
Intent: **in**.
Values: $irst > 0$. This is employed for the BiCGSTABL or RGMRES methods, otherwise it is ignored.

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**.
Intent: **in**.
Values: 1: use the normwise backward error, 2: use the scaled 2-norm of the residual, 3: use the residual reduction in the 2-norm. Default: 2.

On Return

x The computed solution.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type `psb_T_vect_type`.

iter The number of iterations performed.
Scope: **global**
Type: **optional**
Intent: **out**.
Returned as: an integer variable.

err The convergence estimate on exit.
Scope: **global**
Type: **optional**
Intent: **out**.
Returned as: a real number.

cond An estimate of the condition number of matrix A; only available with the CG method on real data.
Scope: **global**
Type: **optional**
Intent: **out**.
Returned as: a real number. A correct result will be greater than or equal to one; if specified for non-real data, or an error occurred, zero is returned.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

11.2 psb_richardson — Richardson Iteration Driver Routine

This subroutine is a driver implementig a Richardson iteration

$$x_{k+1} = M^{-}1(b - Ax_k) + x_k,$$

with the preconditioner operator M defined in the previous section.

The stopping criterion can take the following values:

1 normwise backward error in the infinity norm; the iteration is stopped when

$$err = \frac{\|r_i\|}{(\|A\|\|x_i\| + \|b\|)} < eps$$

2 Relative residual in the 2-norm; the iteration is stopped when

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

3 Relative residual reduction in the 2-norm; the iteration is stopped when

$$err = \frac{\|r_i\|}{\|r_0\|_2} < eps$$

The behaviour is controlled by the istop argument (see later). In the above formulae, x_i is the tentative solution and $r_i = b - Ax_i$ the corresponding residual at the i-th iteration.

```
call psb_richardson(a,prec,b,x,eps,desc_a,info,&
     & itmax,iter,err,itrace,istop)
```

Type: Synchronous.

On Entry

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

prec The data structure containing the preconditioner.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_Tprec_type.

b The RHS vector.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a rank one array or an object of type psb_T_vect_type.

x The initial guess.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type psb_T_vect_type.

eps The stopping tolerance.
Scope: **global**
Type: **required**
Intent: **in**.
Specified as: a real number.

desc_a contains data structures for communications.
Scope: **local**
Type: **required**
Intent: **in**.
Specified as: a structured data of type psb_desc_type.

itmax The maximum number of iterations to perform.
Scope: **global**
Type: **optional**
Intent: **in**.
Default: $itmax = 1000$.
Specified as: an integer variable $itmax \geq 1$.

itrace If > 0 print out an informational message about convergence every *itrace* iterations. If $= 0$ print a message in case of convergence failure.
Scope: **global**
Type: **optional**
Intent: **in**.
Default: $itrace = -1$.

istop An integer specifying the stopping criterion.
Scope: **global**
Type: **optional**.
Intent: **in**.
Values: 1: use the normwise backward error, 2: use the scaled 2-norm of the residual, 3: use the residual reduction in the 2-norm. Default: 2.

On Return

x The computed solution.
Scope: **local**
Type: **required**
Intent: **inout**.
Specified as: a rank one array or an object of type psb_T_vect_type.

iter The number of iterations performed.
Scope: **global**
Type: **optional**
Intent: **out**.
Returned as: an integer variable.

err The convergence estimate on exit.
Scope: **global**
Type: **optional**
Intent: **out**.
Returned as: a real number.

info Error code.
Scope: **local**
Type: **required**
Intent: **out**.
An integer value; 0 means no error has been detected.

12 Extensions

The EXT, CUDA and RSB subdirectories contains a set of extensions to the base library. The extensions provide additional storage formats beyond the ones already contained in the base library, as well as interfaces to:

SPGPU a CUDA library originally published as https://code.google.com/p/spgpu/ and now included in the cuda subdir, for computations on NVIDIA GPUs;

LIBRSB http://sourceforge.net/projects/librsb/, for computations on multicore parallel machines.

The infrastructure laid out in the base library to allow for these extensions is detailed in the references [21, 22, 11]; the CUDA-specific data formats are described in [23].

12.1 Using the extensions

A sample application using the PSBLAS extensions will contain the following steps:

- USE the appropriat modules (psb_ext_mod, psb_cuda_mod);
- Declare a *mold* variable of the necessary type (e.g. psb_d_ell_sparse_mat, psb_d_hlg_sparse_mat, psb_d_vect_cuda);
- Pass the mold variable to the base library interface where needed to ensure the appropriate dynamic type.

Suppose you want to use the CUDA-enabled ELLPACK data structure; you would use a piece of code like this (and don't forget, you need CUDA-side vectors along with the matrices):

```
program my_cuda_test
  use psb_base_mod
  use psb_util_mod
  use psb_ext_mod
  use psb_cuda_mod
  type(psb_dspmat_type) :: a, agpu
  type(psb_d_vect_type) :: x, xg, bg

  real(psb_dpk_), allocatable :: xtmp(:)
  type(psb_d_vect_cuda)       :: vmold
  type(psb_d_elg_sparse_mat) :: aelg
  type(psb_ctxt_type) :: ctxt
  integer             :: iam, np


  call psb_init(ctxt)
  call psb_info(ctxt,iam,np)
  call psb_cuda_init(ctxt, iam)
```

```
  ! My own home-grown matrix generator
  call gen_matrix(ctxt,idim,desc_a,a,x,info)
  if (info /= 0) goto 9999

  call a%cscnv(agpu,info,mold=aelg)
  if (info /= 0) goto 9999
  xtmp = x%get_vect()
  call xg%bld(xtmp,mold=vmold)
  call bg%bld(size(xtmp),mold=vmold)

  ! Do sparse MV
  call psb_spmm(done,agpu,xg,dzero,bg,desc_a,info)


9999 continue
  if (info == 0) then
     write(*,*) '42'
  else
     write(*,*) 'Something went wrong ',info
  end if


  call psb_cuda_exit()
  call psb_exit(ctxt)
  stop
end program my_cuda_test
```

A full example of this strategy can be seen in the `test/ext/kernel` and `test/cuda/kernel` subdirectories, where we provide sample programs to test the speed of the sparse matrix-vector product with the various data structures included in the library.

12.2 Extensions' Data Structures

Access to the facilities provided by the EXT library is mainly achieved through the data types that are provided within. The data classes are derived from the base classes in PSBLAS, through the Fortran 2003 mechanism of *type extension* [18].

The data classes are divided between the general purpose CPU extensions, the GPU interfaces and the RSB interfaces. In the description we will make use of the notation introduced in Table 22.

12.3 CPU-class extensions

ELLPACK

The ELLPACK/ITPACK format (shown in Figure 6) comprises two 2-dimensional arrays `AS` and `JA` with `M` rows and `MAXNZR` columns, where `MAXNZR` is the maximum number of nonzeros in any row [**?**]. Each row of the arrays `AS` and `JA` contains the coefficients and column indices; rows shorter than `MAXNZR` are padded with zero coefficients and appropriate column indices, e.g. the last valid one found in the same row.

Table 22: Notation for parameters describing a sparse matrix

Name	Description
M	Number of rows in matrix
N	Number of columns in matrix
NZ	Number of nonzeros in matrix
AVGNZR	Average number of nonzeros per row
MAXNZR	Maximum number of nonzeros per row
NDIAG	Numero of nonzero diagonals
AS	Coefficients array
IA	Row indices array
JA	Column indices array
IRP	Row start pointers array
JCP	Column start pointers array
NZR	Number of nonzeros per row array
OFFSET	Offset for diagonals

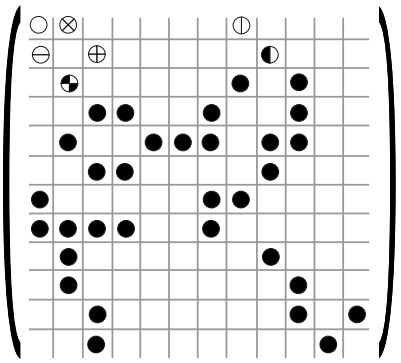

Figure 5: Example of sparse matrix

The matrix-vector product $y = Ax$ can be computed with the code shown in Alg. 1; it costs one memory write per outer iteration, plus three memory reads and two floating-point operations per inner iteration.

Unless all rows have exactly the same number of nonzeros, some of the coefficients in the `AS` array will be zeros; therefore this data structure will have an overhead both in terms of memory space and redundant operations (multiplications by zero). The overhead can be acceptable if:

1. The maximum number of nonzeros per row is not much larger than the average;

2. The regularity of the data structure allows for faster code, e.g. by allowing vectorization, thereby offsetting the additional storage requirements.

In the extreme case where the input matrix has one full row, the ELLPACK structure would require more memory than the normal 2D array storage. The ELLPACK storage format was very popular in the vector computing days; in modern CPUs it is not quite as popular, but it is the basis for many GPU formats.

The relevant data type is `psb_T_ell_sparse_mat`:

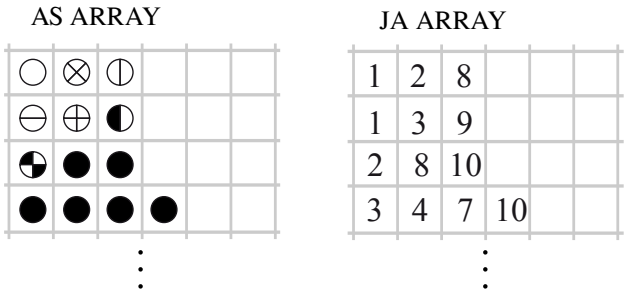

Figure 6: ELLPACK compression of matrix in Figure 5

```
do i=1,n
  t=0
  do j=1,maxnzr
    t = t + as(i,j)*x(ja(i,j))
  end do
  y(i) = t
end do
```

Algorithm 1: Matrix-Vector product in ELL format

```
type, extends(psb_d_base_sparse_mat) :: psb_d_ell_sparse_mat
  !
  ! ITPACK/ELL format, extended.
  !

  integer(psb_ipk_), allocatable :: irn(:), ja(:,:), idiag(:)
  real(psb_dpk_), allocatable :: val(:,:)

contains
  ....
end type psb_d_ell_sparse_mat
```

Hacked ELLPACK

The *hacked ELLPACK* (**HLL**) format alleviates the main problem of the ELLPACK format, that is, the amount of memory required by padding for sparse matrices in which the maximum row length is larger than the average.

The number of elements allocated to padding is $[(m * maxNR) - (m * avgNR) = m * (maxNR - avgNR)]$ for both `AS` and `JA` arrays, where m is equal to the number of rows of the matrix, $maxNR$ is the maximum number of nonzero elements in every row and $avgNR$ is the average number of nonzeros. Therefore a single densely populated row can seriously affect the total size of the allocation.

To limit this effect, in the HLL format we break the original matrix into equally sized groups of rows (called *hacks*), and then store these groups as independent matrices in ELLPACK format. The groups can be arranged selecting rows in an arbitrarily manner; indeed, if the rows are sorted by decreasing

number of nonzeros we obtain essentially the JAgged Diagonals format. If the rows are not in the original order, then an additional vector *rIdx* is required, storing the actual row index for each row in the data structure.

The multiple ELLPACK-like buffers are stacked together inside a single, one dimensional array; an additional vector *hackOffsets* is provided to keep track of the individual submatrices. All hacks have the same number of rows *hackSize*; hence, the *hackOffsets* vector is an array of $(m/hackSize)+1$ elements, each one pointing to the first index of a submatrix inside the stacked cM/rP buffers, plus an additional element pointing past the end of the last block, where the next one would begin. We thus have the property that the elements of the k-th *hack* are stored between `hackOffsets[k]` and `hackOffsets[k+1]`, similarly to what happens in the CSR format.

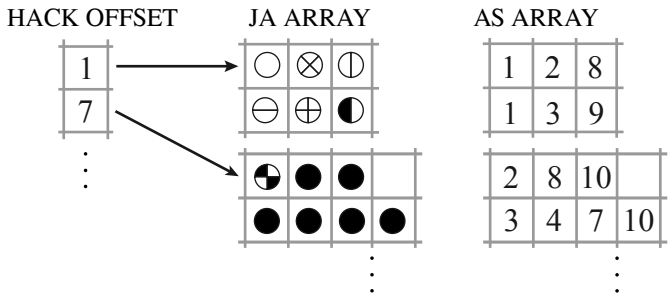

Figure 7: Hacked ELLPACK compression of matrix in Figure 5

With this data structure a very long row only affects one hack, and therefore the additional memory is limited to the hack in which the row appears.

The relevant data type is `psb_T_hll_sparse_mat`:

```
type, extends(psb_d_base_sparse_mat) :: psb_d_hll_sparse_mat
  !
  ! HLL format. (Hacked ELL)
  !
  integer(psb_ipk_) :: hksz
  integer(psb_ipk_), allocatable :: irn(:), ja(:), idiag(:),
   ↪  hkoffs(:)
  real(psb_dpk_), allocatable :: val(:)

contains
 ....
end type
```

Diagonal storage

The DIAgonal (DIA) format (shown in Figure 8) has a 2-dimensional array `AS` containing in each column the coefficients along a diagonal of the matrix, and an integer array `OFFSET` that determines where each diagonal starts. The diagonals in `AS` are padded with zeros as necessary.

The code to compute the matrix-vector product $y = Ax$ is shown in Alg. 2; it costs one memory read per outer iteration, plus three memory reads, one

memory write and two floating-point operations per inner iteration. The accesses to AS and x are in strict sequential order, therefore no indirect addressing is required.

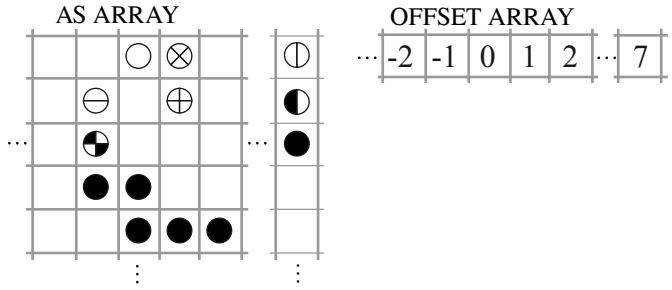

Figure 8: DIA compression of matrix in Figure 5

```
    do j=1,ndiag
      if (offset(j) > 0) then
        ir1 = 1; ir2 = m - offset(j);
      else
        ir1 = 1 - offset(j); ir2 = m;
      end if
      do i=ir1,ir2
        y(i) = y(i) + alpha*as(i,j)*x(i+offset(j))
      end do
    end do
```

Algorithm 2: Matrix-Vector product in DIA format

The relevant data type is `psb_T_dia_sparse_mat`:

```
type, extends(psb_d_base_sparse_mat) :: psb_d_dia_sparse_mat
  !
  ! DIA format, extended.
  !

  integer(psb_ipk_), allocatable :: offset(:)
  integer(psb_ipk_) :: nzeros
  real(psb_dpk_), allocatable :: data(:,:)

end type
```

Hacked DIA

Storage by DIAgonals is an attractive option for matrices whose coefficients are located on a small set of diagonals, since they do away with storing explicitly the indices and therefore reduce significantly memory traffic. However, having a few coefficients outside of the main set of diagonals may significantly increase

the amount of needed padding; moreover, while the DIA code is easily vectorized, it does not necessarily make optimal use of the memory hierarchy. While processing each diagonal we are updating entries in the output vector y, which is then accessed multiple times; if the vector y is too large to remain in the cache memory, the associated cache miss penalty is paid multiple times.

The *hacked DIA* (**HDIA**) format was designed to contain the amount of padding, by breaking the original matrix into equally sized groups of rows (*hacks*), and then storing these groups as independent matrices in DIA format. This approach is similar to that of HLL, and requires using an offset vector for each submatrix. Again, similarly to HLL, the various submatrices are stacked inside a linear array to improve memory management. The fact that the matrix is accessed in slices helps in reducing cache misses, especially regarding accesses to the vector y.

An additional vector *hackOffsets* is provided to complete the matrix format; given that *hackSize* is the number of rows of each hack, the *hackOffsets* vector is made by an array of $(m/hackSize) + 1$ elements, pointing to the first diagonal offset of a submatrix inside the stacked *offsets* buffers, plus an additional element equal to the number of nonzero diagonals in the whole matrix. We thus have the property that the number of diagonals of the *k*-th *hack* is given by *hackOffsets[k+1] - hackOffsets[k]*.

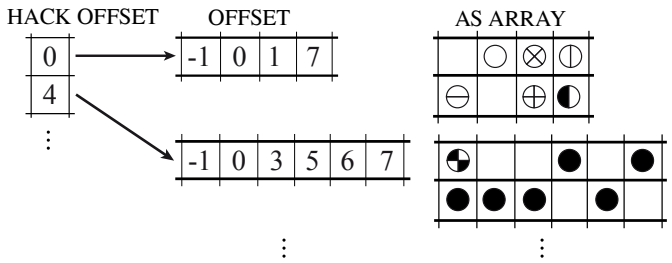

Figure 9: Hacked DIA compression of matrix in Figure 5

The relevant data type is `psb_T_hdia_sparse_mat`:

```
type pm
   real(psb_dpk_), allocatable  :: data(:,:)
end type pm

type po
   integer(psb_ipk_), allocatable  :: off(:)
end type po

type, extends(psb_d_base_sparse_mat) :: psb_d_hdia_sparse_mat
  !
  ! HDIA format, extended.
  !

  type(pm), allocatable :: hdia(:)
  type(po), allocatable :: offset(:)
  integer(psb_ipk_) :: nblocks, nzeros
  integer(psb_ipk_) :: hack = 64
```

```
  integer(psb_long_int_k_) :: dim=0

contains
 ....
end type
```

12.4 CUDA-class extensions

For computing with CUDA we define a dual memorization strategy in which each variable on the CPU ("host") side has a GPU ("device") side. When a GPU-type variable is initialized, the data contained is (usually) the same on both sides. Each operator invoked on the variable may change the data so that only the host side or the device side are up-to-date.

Keeping track of the updates to data in the variables is essential: we want to perform most computations on the GPU, but we cannot afford the time needed to move data between the host memory and the device memory because the bandwidth of the interconnection bus would become the main bottleneck of the computation. Thus, each and every computational routine in the library is built according to the following principles:

- If the data type being handled is GPU-enabled, make sure that its device copy is up to date, perform any arithmetic operation on the GPU, and if the data has been altered as a result, mark the main-memory copy as outdated.
- The main-memory copy is never updated unless this is requested by the user either

  explicitly by invoking a synchronization method;

  implicitly by invoking a method that involves other data items that are not GPU-enabled, e.g., by assignment ov a vector to a normal array.

In this way, data items are put on the GPU memory "on demand" and remain there as long as "normal" computations are carried out. As an example, the following call to a matrix-vector product

```
call psb_spmm(alpha,a,x,beta,y,desc_a,info)
```

will transparently and automatically be performed on the GPU whenever all three data inputs `a`, `x` and `y` are GPU-enabled. If a program makes many such calls sequentially, then

- The first kernel invocation will find the data in main memory, and will copy it to the GPU memory, thus incurring a significant overhead; the result is however *not* copied back, and therefore:
- Subsequent kernel invocations involving the same vector will find the data on the GPU side so that they will run at full speed.

For all invocations after the first the only data that will have to be transferred to/from the main memory will be the scalars `alpha` and `beta`, and the return code `info`.

Vectors: The data type `psb_T_vect_gpu` provides a GPU-enabled extension of the inner type `psb_T_base_vect_type`, and must be used together with the other inner matrix type to make full use of the GPU computational capabilities;

CSR: The data type `psb_T_csrg_sparse_mat` provides an interface to the GPU version of CSR available in the NVIDIA CuSPARSE library;

HYB: The data type `psb_T_hybg_sparse_mat` provides an interface to the HYB GPU storage available in the NVIDIA CuSPARSE library. The internal structure is opaque, hence the host side is just CSR; the HYB data format is only available up to CUDA version 10.

ELL: The data type `psb_T_elg_sparse_mat` provides an interface to the ELLPACK implementation from SPGPU;

HLL: The data type `psb_T_hlg_sparse_mat` provides an interface to the Hacked ELLPACK implementation from SPGPU;

HDIA: The data type `psb_T_hdiag_sparse_mat` provides an interface to the Hacked DIAgonals implementation from SPGPU;

13 CUDA Environment Routines

psb_cuda_init — Initializes PSBLAS-CUDA environment

```
call psb_cuda_init(ctxt [, device])
```

This subroutine initializes the PSBLAS-CUDA environment.

Type: Synchronous.

On Entry

device ID of CUDA device to attach to.
Scope: **local**.
Type: **optional**.
Intent: **in**.
Specified as: an integer value. Default: use `mod(iam,ngpu)` where `iam` is the calling process index and `ngpu` is the total number of CUDA devices available on the current node.

Notes

1. A call to this routine must precede any other PSBLAS-CUDA call.

psb_cuda_exit — Exit from PSBLAS-CUDA environment

```
call psb_cuda_exit(ctxt)
```

This subroutine exits from the PSBLAS CUDA context.

Type: Synchronous.

On Entry

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

psb_cuda_DeviceSync — Synchronize CUDA device

```
call psb_cuda_DeviceSync()
```

This subroutine ensures that all previosly invoked kernels, i.e. all invocation of CUDA-side code, have completed.

psb_cuda_getDeviceCount

```
ngpus =  psb_cuda_getDeviceCount()
```

Get number of devices available on current computing node.

psb_cuda_getDevice

```
ngpus =  psb_cuda_getDevice()
```

Get device in use by current process.

psb_cuda_setDevice

```
info = psb_cuda_setDevice(dev)
```

Set device to be used by current process.

psb_cuda_DeviceHasUVA

```
hasUva = psb_cuda_DeviceHasUVA()
```

Returns true if device currently in use supports UVA (Unified Virtual Addressing).

psb_cuda_WarpSize

```
nw = psb_cuda_WarpSize()
```

Returns the warp size.

psb_cuda_MultiProcessors

```
nmp = psb_cuda_MultiProcessors()
```

Returns the number of multiprocessors in the CUDA device.

psb_cuda_MaxThreadsPerMP

```
nt = psb_cuda_MaxThreadsPerMP()
```

Returns the maximum number of threads per multiprocessor.

psb_cuda_MaxRegistersPerBlock

```
nr = psb_cuda_MaxRegistersPerBlock()
```

Returns the maximum number of register per thread block.

psb_cuda_MemoryClockRate

```
cl = psb_cuda_MemoryClockRate()
```

Returns the memory clock rate in KHz, as an integer.

psb_cuda_MemoryBusWidth

```
nb = psb_cuda_MemoryBusWidth()
```

Returns the memory bus width in bits.

psb_cuda_MemoryPeakBandwidth

```
bw = psb_cuda_MemoryPeakBandwidth()
```

Returns the peak memory bandwidth in MB/s (real double precision).

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