PSBLAS-KINSOL interface

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1 The logic behind a PSBLAS instrumented application

The main aim of the PSBLAS library is the parallel implementation of iterative solvers for sparse linear systems,

$$A\mathbf{x} = \mathbf{b}, \qquad A \in \mathbb{K}^{n \times n}, \qquad \mathbb{K} = \mathbb{R}, \mathbb{C},$$
 (1)

through the distributed memory paradigm operating with message passing. The library includes all the needed routines for this task, e.g, functions for multiplying sparse matrices by dense matrices, for solving block diagonal systems with triangular diagonal entries or for preprocessing sparse matrices.

The pivotal choice to be made in this setting regards the distribution of

the coefficient matrix A for the linear system (1). In PSBLAS this choice is based on the **owner computes rule**: each unknown is assigned to a process that will own the corresponding row in the coefficient matrix and

will carry out all related computations.

If A is obtained from the discretization of a Partial Differential Equation (PDE), this allocation strategy is equivalent to the choice of a partition of the mesh into sub-domains.

! → PSBLAS supports *any* distribution that keeps together the coefficients of each matrix row there are **no other** constraints on the variable assignment.

Any PSBLAS application will always start with the construction of the parallel environment, i.e., of an MPI (virtual) parallel machine, that we call here context by means of the psb_c_init function as

```
psb_i_t ictxt , iam , np;
ictxt = psb_c_init();
psb_c_info(ictxt ,&iam ,&np);
```

that creates a parallel environment on np processors $0, \ldots, np-1$, of which we are process iam.

The next step is represented by the need of subdividing the index space among processes, and this creates a mapping from the "global" numbering $1, \ldots, n$ to a "local" numbering in each process. This means that each process i will own a certain subset $1, \ldots, n_{\text{TOW}_i}$, each element of which corresponds to a certain element of $1 \ldots n$.

Therefore, after the initialization the first step is to establish an index space, and this is done with a call to one of the variants of the psb_cdall function to allocate a descriptor object psb_c_descriptor:

psb_c_cdall_vg :

the association between an index and a process is specified via an integer vector vg[], each index $i \in \{1, ..., ng\}$ is assigned to process vg[i]. The vector vg[] must be identical on all calling processes, and its entries have the ranges (0, ..., np-1) or (1, ..., np) according to the fact that $psb_c_set_index_base(0)$ or $psb_c_set_index_base(1)$ has been called at the beginning. The size ng is specified one can chose to use the entire vector vg[], thus having vg[ng].

Prototype

psb_c_cdall_vg(psb_l_t ng,psb_i_t *vg,psb_i_t ictxt,psb_c_descriptor *cdh);

psb_c_cdall_vl |:

the association is done by specifying the list of indices vl[nl] assigned to the current process; thus, the global problem size nl is given by the range of the aggregate of the individual vectors vl[] specified in the calling processes. The subroutine will check how many times

Owner computes rule

each entry in the global index space (1, ..., nl) is specified in the input lists vl[], therefore it allows for the presence of overlap in the input, and checks for the "orphan" indices.

Prototype

```
psb_c_cdall_vl(psb_i_t nl, psb_l_t *vl, psb_i_t ictxt, psb_c_descriptor *cdh);
```

psb_c_cdall_nl :

produces a generalized block-row distribution of the number of indices belonging to the current process in which each process i gets assigned a consecutive chunk of nl global indices,

Prototype

```
psb_c_cdall_nl (psb_i_t nl, psb_i_t ictxt, psb_c_descriptor *cdh);
```

for the case of a simple minded block distribution, i.e., the index space is first numbered sequentially in a standard way, then the corresponding vector is distributed according to a block distribution directive.

We consider as example the finite difference discretization of the following boundary value problem

$$-\frac{b_1\partial^2 u}{\partial x^2} - \frac{b_2\partial^2 u}{\partial y^2} + \frac{a_1\partial u}{\partial x} + \frac{a_2\partial u}{\partial y} + a_3u = 0, \qquad (x, y, z) \in [0, 1]^3,$$

with Dirichlet boundary conditions, on a uniform grid with idim node per size. All the allocation procedure can be expressed as

```
psb_c_descriptor *cdh;
psb_i_t idim, nb, nlr, nl;
psb_l_t i,ng, *vl, k;
cdh=psb_c_new_descriptor();
psb_c_set_index_base(0);
/* Simple minded BLOCK data distribution */
ng = ((psb_l_t) idim)*idim*idim;
nb = (ng+np-1)/np;
nl = nb;
, nl);
if ((vl=malloc(nb*sizeof(psb_l_t)))=NULL) {
  fprintf(stderr,"On %d: malloc failure\n",iam);
  psb_c_abort(ictxt);
i = ((psb_l_t)iam) * nb;
for (k=0; k< n1; k++)
  vl[k] = i+k;
```

Now that the initial distribution of the index space has been performed, we need to allocate dense vectors and sparse matrices on such index space, and thus we define the complete topology of our computational problem. Since our task is to use the capabilities of SUNDIALS-KINSOL to solve for nonlinear problems, here lies the core of the interfacing between the two codes. In the next two Sections 2, and Section 3 we describe such encapsulation for dense vector, and sparse matrices. Then in Section 4 we describe the interfacing with the **linear solvers** and **preconditioners**

Complete information on the PSBLAS data structures, and functions that are mentioned along the text can be found in [2].

2 The NVECTOR_PSBLAS implementation

The NVECTOR_PSBLAS implementation of the SUNDIALS NVECTOR module provides an interface to the PSBLAS code for handling distributed dense vectors. It defines the *content* field of N_Vector to be a structure containing the PSBLAS descriptor for the data distribution, a PSBLAS vector of double, and the PSBLAS communicator (context).

! All the vectors that have to interact needs to be instantiated on the same parallel context ictxt, and on the same data distribution cdh.

The header file to include when using this module is nvector_psblas.h. The installed module library to link to is sundials_nvecpsblas.lib where .lib is typically .so for shared libraries and .a for static libraries.

2.1 NVECTOR_PSBLAS accessor macros

The following macros are provided to access the content of a NVEC-TOR_PSBLAS vector. The suffix _P in the names denotes the fact that the data are in distributed memory.

NV_CONTENT_P(v) this macro gives access to the contents of the PSBLAS vector N_Vector.

NV_DESCRIPTOR_P(v), NV_OWN_DATA_P(v), NV_PVEC_P(v) these macros give instead individual access to the parts of the content of a PSBLAS parallel ${\tt N_Vector}.$

this macro provides the PSBLAS context used by the NVECTOR_PSBLAS vectors.

2.2 NVECTOR_PSBLAS functions

NV_ICTXT_P(v)

The NVECTOR_PSBLAS implementation provides PSBLAS implementations of all the vectors operations listed in Tables 6.2, 6.3, and 6.4 of the original KINSOL library [1]. Following the standard nomenclature of the SUNDIALS library, their names are obtained from the ones listed in Tables 6.2, 6.3, and 6.4 by appending the suffix _PSBLAS. The NVECTOR_PSBLAS implementation provides the following additional user-callable routines.

N_VNew_PSBLAS : This function creates and allocates memory for a parallel vector on the PSBLAS context ictxt with the communicator cdh

Prototype N_Vector N_VNew_PSBLAS(int ictxt, psb_c_descriptor *cdh);

N_VNewEmpty_PSBLAS: This function creates a new PSBLAS vector with empty data array.

Prototype N_Vector N_VNewEmpty_PSBLAS(int ictxt, psb_c_descriptor *cdh);

N_VMake_PSBLAS : Function to

Function to create a PSBLAS N_{vector} with user data component. This function is substantially a wrapper for the PSBLAS function psb_c_dgeins.

Prototype

N_Vector N_VMake_PSBLAS(int ictxt, psb_c_descriptor *cdh,psb_i_t m, psb_i_t *irow,double *val);

The PSBLAS context ictxt with the communicator cdh are the one defined for the whole programs, the integer m is the number of rows in val [] to be inserted, the array of integers irow is the indices of the rows to be inserted. Specifically, row i of val will be inserted into the local row corresponding to the global index row index row[i].

 $! \rightarrow$

This routine does not assemble the final vector. After the insertion of all the elements has been completed then the vector should be assembled by means of the N_VAsb_PSBLAS routine.

N_VAsb_PSBLAS :

This routine assemble the NVector after that all the elements have been inserted into it, i.e., after that all the calls to the N_VMake_PSBLAS routine have been completed. This is substantially a wrapper for the PSBLAS function psb_c_dgeasb.

Prototype

void N_VAsb_PSBLAS(N_Vector v)

N_VCloneVectorArray_PSBLAS | :

This function creates an array of new parallel vectors (by cloning) an array of count parallel vectors v.

an array of count paramet vectors v.

Prototype

N_VCloneVectorArrayEmpty_PSBLAS :

S: This function creates an array of count new parallel vectors with empty data array on the same communicator and context of the vector w.

Prototype

N_Vector *N_VCloneVectorArrayEmpty_PSBLAS(int count, N_Vector w)

N_VDestroyVectorArray_PSBLAS

This function to frees an array of count N_Vectors created with N_VCloneVectorArray_PSBLAS

Prototype

void N_VDestroyVectorArray_PSBLAS(N_Vector *vs, int count)

N_VGetLength_PSBLAS :

This function returns the *global* vector length, this is substantially a wrapper for the PSBLAS function psb_c_cd_get_global_rows.

Prototype

 $sunindextype \ N_VGetLength_PSBLAS(N_Vector \ v)$

N_VGetLocalLength_PSBLAS

This function returns the *local* vector length, this is substantially a wrapper for the PSBLAS function psb_c_cd_get_local_rows.

Prototype

sunindextype N_VGetLocalLength_PSBLAS(N_Vector v)

N_VPrint_PSBLAS :

This function prints the local data in a parallel vector to stdout.

Prototype

void N_VPrint_PSBLAS(N_Vector x)

N_VPrintFile_PSBLAS :

This function prints the local data in a parallel vector to outfile.

Prototype

void N_VPrintFile_PSBLAS(N_Vector x, FILE* outfile)

N_VGetVectorID_PSBLAS :

This function returns the SUNDIALS identificative for the PSBLAS vector, since this is a custom implementation it returns the integer constant SUNDIALS_NVEC_CUSTOM.

Prototype

N_Vector_ID N_VGetVectorID_PSBLAS(N_Vector v)

N_VCloneEmpty_PSBLAS

Clones a NVECTOR_PSBLAS with a NULL pvec field, and with value SUNFALSE in the own_data field.

Prototype N_Vector N_VCloneEmpty_PSBLAS(N_Vector w)

N_VClone_PSBLAS : Clones a NVECTOR_PSBLAS allocating its memory following the

same communicator of the cloned one.

Prototype N_Vector N_VClone_PSBLAS(N_Vector w)

N_VDestroy_PSBLAS : Destroys a NVECTOR_PSBLAS freeing both the memory allocated

for the corresponding PSBLAS vector, and the memory allocated

for the NVECTOR_PSBLAS structure.

Prototype void N_VDestroy_PSBLAS(N_Vector v)

N_VSpace_PSBLAS : Returns storage requirements for one NVECTOR_PSBLAS. Irw

contains the number of realtype words and liw contains the number

of integer words.

Prototype void N_VSpace_PSBLAS(N_Vector v, sunindextype *lrw,sunindextype *liw)

N_VGetArrayPointer_PSBLAS | : Returns a pointer to a realtype array from the NVECTOR_PSBLAS,

this is the local portion of the distributed PSBLAS vector encap-

sulated in the N_Vector object.

Prototype realtype *N_VGetArrayPointer_PSBLAS(N_Vector v)

N_VSetArrayPointer_PSBLAS : This function is a dummy function, in PSBLAS we use allocatable

objects for the local part of the distributed vector, and, moreover,

we assume having an arbitrary distribution of the indexes.

Prototype void N_VSetArrayPointer_PSBLAS(psb_c_dvector *v_data, N_Vector v)

N_VLinearSum_PSBLAS |: Performs the AXPBY BLAS operation between to NVECTOR_PSBLAS,

the result can be both out-of- and in-place.

Prototype void N_VLinearSum_PSBLAS(realtype a, N_Vector x, realtype b, N_Vector y,

 $N_{\text{-}}Vector z)$

 $\verb|N_VConst_PSBLAS|: Sets all components of the NVECTOR_PSBLAS to a constant value$

and assembles it, the user does not need to assembly it.

Prototype void N_VConst_PSBLAS(realtype c, N_Vector z)

N_VProd_PSBLAS : Performs the entry-wise multiplication of two NVECTOR_PSBLAS,

the result can be both out-of- and in-place.

Prototype void N_VProd_PSBLAS(N_Vector x, N_Vector y, N_Vector z)

N_VDiv_PSBLAS : Performs the entry-wise division of two NVECTOR_PSBLAS, the

result can be both out-of- and in-place, it does not check for possible zero entries in the denumerator. It is up to the user to guarantee

that this does not happens.

Prototype void N_VDiv_PSBLAS(N_Vector x, N_Vector y, N_Vector z)

N_VScale_PSBLAS : Scales an NVECTOR_PSBLAS by a scalar c, the result can be both

out-of- and in-place.

Prototype void N_VScale_PSBLAS(realtype c, N_Vector x, N_Vector z)

N_VAbs_PSBLAS : Sets the entries of an NVECTOR_PSBLAS to the absolute values

of the entries of the input.

 $\label{eq:prototype} Prototype \qquad \qquad \text{void $N_VAbs_PSBLAS}(N_Vector \ x, \ N_Vector \ z)$

N_VInv_PSBLAS : Sets the entries of an NVECTOR_PSBLAS to the inverse of the

entries of the input. It does not check for possible zero entries in

the vector. It is up to the user to guarantee that this does not happens.

----P P --

Prototype void N_VInv_PSBLAS(N_Vector x, N_Vector z)

N_VAddConst_PSBLAS : Adds a scalar to all components of an NVECTOR_PSBLAS and returns the result in another NVECTOR_PSBLAS object.

Prototype void N_VAddConst_PSBLAS(N_Vector x, realtype b, N_Vector z)

N_VDotProd_PSBLAS : Compute the dot product of two NVECTOR_PSBLAS objects.

Prototype realtype N_VDotProd_PSBLAS(N_Vector x, N_Vector y)

N_VMaxNorm_PSBLAS : Compute the max norm of an NVECTOR_PSBLAS object.

Prototype realtype N_VMaxNorm_PSBLAS(N_Vector x)

N_VWrmsNorm_PSBLAS : Compute the weighted (by the size) 2-norm of an NVECTOR_PSBLAS

object.

Prototype realtype N_VWrmsNorm_PSBLAS(N_Vector x, N_Vector w)

N_VWrmsNormMask_PSBLAS : Returns the weighted root mean square norm of the NVEC-

TOR_PSBLAS ${\bf x}$ with real type weight vector ${\bf w}$ built using only the elements of ${\bf x}$ corresponding to positive elements of the NVEC-

TOR_PSBLAS id.

Prototype realtype N_VWrmsNormMask_PSBLAS(N_Vector x,N_Vector w,N_Vector id)

N_VMin_PSBLAS : Gives back the minimum entry of an NVECTOR_PSBLAS object.

Prototype realtype N_VMin_PSBLAS(N_Vector x)

N_VWL2Norm_PSBLAS : Returns the weighted Euclidean 2-norm of the NVECTOR_PSBLAS

x with realtype weight vector w.

Prototype realtype N_VWL2Norm_PSBLAS(N_Vector x, N_Vector w)

N_VL1Norm_PSBLAS : Computes the 1-norm of an NVECTOR_PSBLAS object.

Prototype realtype N_VL1Norm_PSBLAS(N_Vector x)

N_VCompare_PSBLAS : Compares the components of the NVECTOR_PSBLAS x to the

realtype scalar c and returns an NVECTOR_PSBLAS z such that

$$z_i = \begin{cases} 1.0, & |x_i| \ge c, \\ 0.0, & |x_i| \le c. \end{cases}$$

Prototype void N_VCompare_PSBLAS(realtype c, N_Vector x, N_Vector z)

N_VInvTest_PSBLAS : Sets the entries of an NVECTOR_PSBLAS to the inverse of the

entries of the input. It checks for possible zero entries in the vector. This routine returns a boolean assigned to SUNTRUE if all components of the vector are nonzero (successful inversion) and returns

SUNFALSE otherwise.

 $\label{eq:prototype} Prototype & booleantype N_VInvTest_PSBLAS(N_Vector \ x, \ N_Vector \ z) \\$

N_VConstrMask_PSBLAS: Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \ge 0$ if

 $c_i = 1$, $x_i \le 0$ if $c_i = -1$, $x_i < 0$ if $c_i = -2$. There is no constraint on x_i if $c_i = 0$. This routine returns a boolean assigned to SUNFALSE if any element failed the constraint test and assigned to SUNTRUE if all passed. It also sets a mask vector m, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed.

This routine is used only for constraint checking.

Prototype

booleantype N_VConstrMask_PSBLAS(N_Vector c, N_Vector x, N_Vector m)

N_VMinQuotient_PSBLAS

This routine returns the minimum of the quotients obtained by term-wise dividing num[i] by denom[i]. A zero element in denom will be skipped. If no such quotients are found, then the large value BIG REAL (defined in the header file sundials types.h) is returned.

Prototype

realtype N_VMinQuotient_PSBLAS(N_Vector num, N_Vector denom)

2.2.1 Fused operation

N_VLinearCombination_PSBLAS

This routine computes the linear combination of nv vectors with n elements

$$z_i = \sum_{j=0}^{n_v - 1} c_j x_{j,i}, \qquad i = 0, \dots, n - 1$$

where c is an array of nv scalars, X is an array of $NVECTOR_PSBLAS$. When z is one of the vectors in X, then it is assumed to be the first vector in the vector array.

Prototype

int N_VLinearCombination_PSBLAS(int nvec, realtype* c, N_Vector* V,N_Vector z)

N_VScaleAddMulti_PSBLAS :

This routine scales and adds one vector to nv vectors with n elements:

$$z_{j,i} = c_j x_i + y_{j,i}, \qquad j = 0, \dots, n_v - 1, \qquad i = 0, \dots, n - 1,$$

where c is an array of nv scalars.

Prototype

int N_VScaleAddMulti_PSBLAS(int nvec, realtype* a, N_Vector x, N_Vector* Y, N_Vector* Z)

N_VDotProdMulti_PSBLAS

This routine computes the dot product of a vector with nv other vectors.

Prototype

int N_VDotProdMulti_PSBLAS(int nvec, N_Vector x,N_Vector *Y, realtype* dotprods)

2.2.2 Vector array operations

 ${\tt N_VLinearSumVectorArray_PSBLAS}$:

This routine computes the linear sum of two vector arrays containing nv vectors of n elements:

$$z_{j,i} = ax_{j,i} + by_{j,i},$$
 $i = 0, \dots, n-1,$ $j = 0, \dots, n_v - 1.$

Prototype

int N_VLinearSumVectorArray_PSBLAS(int nvec, realtype a, N_Vector* X, realtype b, N_Vector* Y, N_Vector* Z)

N_VScaleVectorArray_PSBLAS :

This routine scales each vector of n elements in a vector array of n_{-v} vectors by a (potentially different) constant:

$$z_{j,i} = c_j x_{j,i}, \qquad i = 0, \dots, n-1, \qquad j = 0, \dots, n_v - 1.$$

Prototype

int N_VScaleVectorArray_PSBLAS(int nvec, realtype* c,N_Vector* X, N_Vector* Z)

N_VConstVectorArray_PSBLAS :

This routine sets each element in a vector of n elements in a vector array of nv vectors to the same value.

Prototype

int N_VConstVectorArray_PSBLAS(int nvecs, realtype c,N_Vector* Z)

```
N_VWrmsNormVectorArray_PSBLAS : This routine computes the weighted root mean square norm of nv vectors with n elements.

Prototype int N_VWrmsNormVectorArray_PSBLAS(int nvecs, N_Vector* X,N_Vector* W, realtype* nrm)
```

N_VWrmsNormMaskVectorArray_PSBLAS : This routine computes the masked weighted root mean square norm of nv vectors with n elements.

Prototype int N_VWrmsNormMaskVectorArray_PSBLAS(int nvec, N_Vector* X,N_Vector * W, N_Vector id,realtype* nrm)

N_VScaleAddMultiVectorArray_PSBLAS : This routine scales and adds a vector in a vector array of nv vectors to the corresponding vector in ns vector arrays.

Prototype int N_VScaleAddMultiVectorArray_PSBLAS(int nvec, int nsum, realtype* a, N_Vector* X, N_Vector** Y, N_Vector** Z)

N_VLinearCombinationVectorArray_PSBLAS : This routine computes the linear combination of ns vector arrays containing nv vectors with n elements.

Prototype int N_VLinearCombinationVectorArray_PSBLAS(int nvec, int nsum, realtype * c, N_Vector** X, N_Vector** Z)

By default all fused and vector array operations are disabled in the nvector PSBLAS module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector.

```
int N_VEnableFusedOps_PSBLAS(N_Vector v, booleantype tf);
   N_VEnableLinearCombination_PSBLAS(N_Vector v, booleantype
int
int N_VEnableScaleAddMulti_PSBLAS(N_Vector v, booleantype tf);
int N_VEnableDotProdMulti_PSBLAS(N_Vector v, booleantype tf);
   N_VEnableLinearSumVectorArray_PSBLAS(N_Vector v,
    booleantype tf);
int N_VEnableScaleVectorArray_PSBLAS(N_Vector v, booleantype
int N_VEnableConstVectorArray_PSBLAS(N_Vector v, booleantype
int N_VEnableWrmsNormVectorArray_PSBLAS(N_Vector v,
    booleantype tf);
int N_VEnableWrmsNormMaskVectorArray_PSBLAS(N_Vector v,
    booleantype tf);
int \  \, N\_VEnableScaleAddMultiVectorArray\_PSBLAS\,(\, \underbrace{N\_Vector} \  \, v\,,
    booleantype tf);
int N_VEnableLinearCombinationVectorArray_PSBLAS(N_Vector v,
    booleantype tf);
```

3 The SUNMATRIX_PSBLAS implementation

4 The SUNLINSOL_PSBLAS implementation

4.1 Algebraic Multigrid Preconditioners

References

[1] Aaron M. Collier et al. *User Documentation for kinsol v4.1.0*. Center for Applied Scientific Computing Lawrence Livermore National Laboratory. URL: https://computing.llnl.gov/sites/default/files/public/kin_guide.pdf.

[2] S. Filippone and A. Buttari. PSBLAS 3.6.1 User's guide. A reference guide for the Parallel Sparse BLAS library. Cranfield University, Centre for Computational Engineering Sciences. URL: https://github.com/sfilippone/psblas3/blob/development/docs/psblas-3.6.pdf.