

BDDCML

solver library based on Multi-Level Balancing Domain Decomposition by Constraints
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version 2.2

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Table of Contents

1	Introduction.....	1
2	How to use BDDCML.....	2
3	Notes for C/C++ users.....	4
3.1	Header file.....	4
3.2	Cross-compilation.....	4
3.3	Libraries of Fortran compiler.....	4
4	Description of interface functions.....	5
4.1	<code>bddcml_init</code>	5
	C interface.....	5
	Fortran interface.....	5
	Description.....	5
	Parameters.....	5
4.2	<code>bddcml_upload_global_data</code>	7
	C interface.....	7
	Fortran interface.....	7
	Description.....	7
	Parameters.....	8
4.3	<code>bddcml_upload_subdomain_data</code>	10
	C interface.....	10
	Fortran interface.....	10
	Description.....	11
	Parameters.....	11
4.4	<code>bddcml_setup_preconditioner</code>	15
	C interface.....	15
	Fortran interface.....	15
	Description.....	15
	Parameters.....	15
4.5	<code>bddcml_solve</code>	17
	C interface.....	17
	Fortran interface.....	17
	Description.....	17
	Parameters.....	17
4.6	<code>bddcml_download_local_solution</code>	19
	C interface.....	19
	Fortran interface.....	19
	Description.....	19
	Parameters.....	19
4.7	<code>bddcml_download_global_solution</code>	20
	C interface.....	20

Fortran interface	20
Description	20
Parameters	20
4.8 bddcml_download_local_reactions	21
C interface	21
Fortran interface	21
Description	21
Parameters	21
4.9 bddcml_download_global_reactions	22
C interface	22
Fortran interface	22
Description	22
Parameters	22
4.10 bddcml_change_global_data	23
C interface	23
Fortran interface	23
Description	23
Parameters	23
4.11 bddcml_change_subdomain_data	24
C interface	24
Fortran interface	24
Description	24
Parameters	24
4.12 bddcml_setup_new_data	26
C interface	26
Fortran interface	26
Description	26
Parameters	26
4.13 bddcml_dotprod_subdomain	27
C interface	27
Fortran interface	27
Description	27
Parameters	27
4.14 bddcml_finalize	28
C interface	28
Fortran interface	28
Description	28
Parameters	28

1 Introduction

The BDDCML (Balancing Domain Decomposition by Constraints - Multi-Level) is a library for solving large sparse linear systems resulting from computations by the finite element method (FEM). Domain decomposition technique is employed which allows distribution of the computations among processors.

The main goal of the package is to provide a scalable implementation of the (Adaptive) Multilevel BDDC method. Codes are written in Fortran 95 with MPI library. A library is provided, which is supposed to be called from users' applications. It provides a simple interface functions callable from Fortran and C.

Balancing Domain Decomposition by Constraints (BDDC) has quickly evolved into a very popular method. However, for very large numbers of subdomain, the coarse problem becomes a large problem to be solved in its own right. In Multilevel BDDC, the coarse problem is solved only approximately by recursive application of BDDC to higher levels.

The main web site of the BDDCML project is

<http://www.math.cas.cz/~sistek/software/bddcml.html>

In case of questions, reporting a bug, or just of interest, feel free to contact Jakub Šístek at sistek@math.cas.cz.

2 How to use BDDCML

The library provides a simple interface callable from Fortran and C. Although main parts of the solver are purely algebraic, the solver needs also to get some information of the computational mesh. This requirement is mainly motivated by selection of corners within the method, for which existing algorithms rely on geometry.

Two different modes are possible for input:

- user can either provide information about global mesh and a file with element matrices (global loading),
- user can provide division into subdomains on the first level and pass subdomain matrices for each subdomain to the routine (local loading).

The solution process is divided into the following sequence of called functions. Their parameters are described in separate sections.

1. `bddcml_init` – initialization of the solver
2.
 - `bddcml_upload_global_data` – loading global data about computational mesh and matrix (use for global loading)
 - `bddcml_upload_subdomain_data` – loading data for one subdomain mesh and matrix (use for local loading)
3. `bddcml_setup_preconditioner` – prepare preconditioner
4. `bddcml_solve` – solve loaded system by preconditioned Krylov subspace iterative method (PCG or BiCGstab)
5.
 - `bddcml_download_local_solution` – get the solution restricted to a subdomain from the solver (use for local loading)
 - `bddcml_download_global_solution` – get the global solution from the solver (use for global loading)
6. `bddcml_finalize` – clear solver data and deallocate memory

Two examples are presented in the ‘`examples`’ folder. Both are written in Fortran 90. The ‘`bddcml_global.f90`’ demonstrates the use of global input, while the ‘`bddcml_local.f90`’ demonstrates the use of localized subdomain input. Optionally, one can ask for nodal reactions at Dirichlet boundary conditions by

- `bddcml_download_local_reactions` – get the reactions restricted to a subdomain from the solver (use for local loading)
- `bddcml_download_global_reactions` – get the global reactions from the solver (use for global loading)

The solver supports efficient handling of multiple-right hand side, for which the matrix as well as preconditioner are reused. Moreover, the Krylov method is accelerated by storing some of the Krylov basis. One can re-run the Krylov method for a new right-hand side and/or values of Dirichlet boundary conditions as

1.
 - `bddcml_change_global_data` – changing global data about right-hand side or Dirichlet b.c. (use for global loading)
 - `bddcml_change_subdomain_data` – changing data for one subdomain about right-hand side or Dirichlet b.c. (use for local loading)
2. `bddcml_setup_new_data` – after right-hand side or Dirichlet b.c. has changed, recreate related internal arrays
3. `bddcml_solve` – solve the system again for the new data

3 Notes for C/C++ users

Since BDDCML is written in Fortran 95 language, users who want to use BDDCML from C/C++ need to overcome a few issues related to this fact.

3.1 Header file

There is a C interface provided in the file `'bddcml_interface_c.h'` that has to be included in applications. In C++, users should include this file using the `extern` directive as

```
extern "C" {  
    #include <bddcml_interface_c.h>  
}
```

3.2 Cross-compilation

Fortran compilers change the name of subroutines as they appear in the code when they generate symbols out of them (this is mainly related to historical reasons). Some Fortran compilers append `'_'` at the end of the name, some append `'__'`, some do not do anything to the name and some change all letters to upper case. In order to combine C and Fortran code, it is necessary to mimic the behaviour of the Fortran compiler in a C/C++ code by modifying names of the C functions (both when calling Fortran routine from a C function and vice versa). For a somewhat generic behaviour of this naming convention, there is an `F_SYMBOL` macro defined in `'bddcml_interface_c.h'` which changes the C names to match the name expected by Fortran. This is based on a preprocessor variable used in compiling C/C++ code. Possible values include:

- `Add_` - append `'_'` at the end of the function name (this is most common and used e.g. by `gfortran` or `Intel Fortran Compiler`)
- `Add__` - append `'__'` at the end of the function name (used e.g. by `g95`)
- `UPPER` - change all letters to uppercase

This should appear on command line as e.g. `-DAdd_` during compiling. If nothing is defined, no change is done to the symbol name, which is in fact correct for certain Fortran compilers, such as those by IBM.

3.3 Libraries of Fortran compiler

If C code is called from Fortran, no additional libraries are usually needed. However, in the opposite case, i.e. the one encountered if BDDCML is used from a C/C++ code, one needs to explicitly specify the libraries of Fortran compiler in the linking sequence when the final executable is build by a C++ linker. For example, if combining `g++` and `gfortran`, it is necessary to add

```
-L/usr/lib -lmpi_f77 -lgfortran
```

when linking an executable by `g++`. Obviously, the path may be different from this example on a particular machine.

4 Description of interface functions

In this chapter, detailed description of the solver interface functions with explanation of individual arguments is given

4.1 bddcml_init

C interface

```
void bddcml_init( int *nl, int *nsublev, int *lnsublev, int *nsub_loc_1, int
*comm_init, int *verbose_level, int *numbase );
```

Fortran interface

```
subroutine bddcml_init(nl, nsublev,lnsublev, nsub_loc_1, comm_init,
verbose_level, numbase)
```

```
    integer, intent(in) :: nl
    integer, intent(in) :: lnsublev
    integer, intent(in) :: nsublev(lnsublev)
    integer, intent(inout):: nsub_loc_1
    integer, intent(in):: comm_init
    integer, intent(in):: verbose_level
    integer, intent(in) :: numbase
```

Description

Prepares internal data structures for the solver.

Parameters

- nl** given number of levels, $nl \geq 2$, $nl = 2$ corresponds to standard (two-level) BDDC method
- nsublev** array with GLOBAL numbers of subdomains for each level. Need to be monotonically decreasing from $nsublev(1) = \text{sum}(nsub_loc_1)$ to $nsublev(nl) = 1$
- lnsublev** length of array **nsublev** - should match **nl**
- nsub_loc_1** LOCAL number of subdomains assigned to the process.
- ≥ 0 number of local subdomains - sum up across processes to $nsublev[0]$
 - -1 let solver decide, the value is returned (determining linear partition)
- comm_init** initial global communicator (possibly `MPI_COMM_WORLD`). This should be communicator in Fortran. When called from C, it should NOT be of type `MPI_Comm` but of type `int *`, and user should use the `MPI_Comm_c2f` function to convert the C `MPI_Comm` communicator to Fortran communicator of type `int *`.
- verbose_level** level of verbosity

- 0 - only errors printed
- 1 - some output
- 2 - detailed output

numbase first index of arrays (0 for C, 1 for Fortran)

4.2 bddcml_upload_global_data

C interface

```
void bddcml_upload_global_data( int *nelem, int *nnod, int *ndof, int *ndim,
int *meshdim, int *inet, int *linet, int *nnet, int *lnnet, int *nndf, int
*lnndf, double *xyz, int *lxyz1, int *lxyz2, int *ifix, int *lifix, double
*fixv, int *lfixv, double *rhs, int *lrhs, double *sol, int *lsol, int *idelm,
int *neighbouring, int *load_division_int );
```

Fortran interface

```
subroutine bddcml_upload_global_data(nelem,nnod,ndof,ndim,meshdim,&
inet,linet,nnet,lnnet,nndf,lnndf,xyz,lxyz1,lxyz2,& ifix,lifix, fixv,lfixv,
rhs,lrhs, sol,lsol, idelm, & neighbouring, load_division_int)
```

```
integer, intent(in):: nelem
integer, intent(in):: nnod
integer, intent(in):: ndof
integer, intent(in) :: ndim
integer, intent(in) :: meshdim
integer, intent(in):: linet
integer, intent(in):: inet(linet)
integer, intent(in):: lnnet
integer, intent(in):: nnet(lnnet)
integer, intent(in):: lnndf
integer, intent(in):: nndf(lnndf)
integer, intent(in):: lxyz1, lxyz2
real(kr), intent(in):: xyz(lxyz1,lxyz2)
integer, intent(in):: lifix
integer, intent(in):: ifix(lifix)
integer, intent(in):: lfixv
real(kr), intent(in):: fixv(lfixv)
integer, intent(in):: lrhs
real(kr), intent(in):: rhs(lrhs)
integer, intent(in):: lsol
real(kr), intent(in):: sol(lsol)
integer, intent(in) :: idelm
integer, intent(in) :: neighbouring
integer, intent(in) :: load_division_int
```

Description

If no distribution of data exists in the user application, it may be left to the solver. This routine loads global information on mesh connectivity and coordinates. Matrix is passed as unassembled matrices of individual elements which will be read from opened file unit `idelm` and assembled within the solver. If partitioning into subdomains on the basic level exists in user's application, routine `bddcml_upload_subdomain_data` should be used instead.

Parameters

<code>nelem</code>	GLOBAL number of elements
<code>nmod</code>	GLOBAL number of nodes
<code>ndof</code>	GLOBAL number of degrees of freedom, i.e. size of matrix
<code>ndim</code>	number of space dimensions
<code>meshdim</code>	mesh dimension. For 3D elements = <code>ndim</code> , for 3D shells = 2, for 3D beams = 1
<code>inet</code>	GLOBAL array with Indices of Nodes on Elements - this defines connectivity of the mesh.
<code>linet</code>	length of array <code>inet</code> . It is given as a sum of entries in array <code>nnet</code> .
<code>nnet</code>	GLOBAL array with Number of Nodes on Elements. For each element, it gives number of nodes it is connected to. This is important to locate element entries in array <code>inet</code>
<code>lnnet</code>	length of array <code>nnet</code> . It is equal to <code>nelem</code> .
<code>nndf</code>	GLOBAL array with Number of Nodal Degrees of Freedom. For each node, it gives number of attached degrees of freedom.
<code>lnndf</code>	length of array <code>nndf</code> . It is equal to <code>nmod</code> .
<code>xyz</code>	GLOBAL Coordinates of nodes as one array (all X, all Y, all Z) or as two-dimensional array in Fortran (X Y Z). Rows are defined by nodes, columns are defined by dimension.
<code>lxyz1,lxyz2</code>	dimensions of array <code>xyz</code> . In C, length of <code>xyz</code> is defined as <code>lxyz1 * lxyz2</code> . In Fortran, dimension of <code>xyz</code> is given used as <code>xyz(lxyz1,lxyz2)</code> . The <code>lxyz1</code> is equal to <code>nmod</code> . The <code>lxyz2</code> is equal to <code>ndim</code> .
<code>ifix</code>	GLOBAL array of Indices of FIXED variables - all degrees of freedom with Dirichlet boundary condition are marked by 1, degrees of freedom not prescribed are marked by 0, i.e. non-zero entries determine fixed degrees of freedom. The values of prescribed boundary conditions are given by corresponding entries of array <code>fixv</code> .
<code>lifix</code>	length of array <code>ifix</code> , equal to <code>ndof</code> .
<code>fixv</code>	GLOBAL array of FIXED Variables - where <code>ifix</code> is non-zero, <code>fixv</code> stores value of Dirichlet boundary condition. Where <code>ifix</code> is zero, corresponding value in <code>fixv</code> is meaningless.
<code>lfixv</code>	length of array <code>fixv</code> , equal to <code>ndof</code> .
<code>rhs</code>	GLOBAL array with Right-Hand Side
<code>lrhs</code>	length of array <code>rhs</code> , equal to <code>ndof</code> .
<code>sol</code>	GLOBAL array with initial SOLUTION guess. This is used as initial approximation for iterative method.
<code>lsol</code>	length of array <code>sol</code> , equal to <code>ndof</code> .

`idelm` opened Fortran unit with unformatted file with element matrices

`neighbouring`

how many nodes should be shared by two elements to call them adjacent in graph. This parameter is used for division of mesh on the basic level by ParMETIS or METIS. Often, one gets better results if he specifies this number to define adjacency only if elements share a face in 3D or edge in 2D. E.g. for linear tetrahedra, the recommended value is 3.

`load_division_int`

Should division from file '`partition_11.ES`' be used? (0 - partition is created in the solver, 1 - partition is read) If partition is read, the file contains for each element, number of subdomain it belongs to. Begins from 1.

4.3 bddcml_upload_subdomain_data

C interface

```
void bddcml_upload_subdomain_data( int *nelem, int *nnod, int *ndof, int
*ndim, int *meshdim, int *isub, int *nelems, int *nnods, int *ndofs, int *inet,
int *linet, int *nnet, int *lnnet, int *nndf, int *lnndf, int *isngn, int
*lisngn, int *isvgvn, int *lisvgvn, int *isegn, int *lisegn, double *xyz,
int *lxyz1, int *lxyz2, int *ifix, int *lifix, double *fixv, int *lfixv,
double *rhs, int *lrhs, int *is_rhs_complete, double *sol, int *lsol, int
*matrixtype, int *i_sparse, int *j_sparse, double *a_sparse, int *la, int
*is_assembled_int, double *user_constraints, int *luser_constraints1,
int *luser_constraints2, double *element_data, int *lelement_data1, int
*lelement_data2, double *dof_data, int *ldof_data );
```

Fortran interface

```
subroutine bddcml_upload_subdomain_data(nelem, nnod, ndof, ndim, meshdim,
& isub, nelems, nnods, ndofs, & inet, linet, nnet, lnnet, nndf, lnndf, &
isngn, lisngn, isvgvn, lisvgvn, isegn, lisegn, & xyz, lxyz1, lxyz2, & ifix, lifix,
fixv, lfixv, & rhs, lrhs, is_rhs_complete_int, & sol, lsol, & matrixtype,
i_sparse, j_sparse, a_sparse, la, is_assembled_int, & user_constraints, luser_
constraints1, luser_constraints2, & element_data, lelement_data1, lelement_
data2, & dof_data, ldof_data)
```

```
integer, intent(in):: nelem
integer, intent(in):: nnod
integer, intent(in):: ndof
integer, intent(in):: ndim
integer, intent(in):: meshdim
integer, intent(in):: isub
integer, intent(in):: nelems
integer, intent(in):: nnods
integer, intent(in):: ndofs
integer, intent(in):: linet
integer, intent(in):: inet(linet)
integer, intent(in):: lnnet
integer, intent(in):: nnet(lnnet)
integer, intent(in):: lnndf
integer, intent(in):: nndf(lnndf)
integer, intent(in):: lisngn
integer, intent(in):: isngn(lisngn)
integer, intent(in):: lisvgvn
integer, intent(in):: isvgvn(lisvgvn)
integer, intent(in):: lisegn
integer, intent(in):: isegn(lisegn)
integer, intent(in):: lxyz1, lxyz2
real(kr), intent(in):: xyz(lxyz1, lxyz2)
```

```

integer, intent(in):: lifix
integer, intent(in):: ifix(lifix)
integer, intent(in):: lfixv
real(kr), intent(in):: fixv(lfixv)
integer, intent(in):: lrhs
real(kr), intent(in):: rhs(lrhs)
integer, intent(in):: lsol
real(kr), intent(in):: sol(lsol)
integer, intent(in):: is_rhs_complete_int
integer, intent(in):: matrixtype
integer, intent(in):: i_sparse(la)
integer, intent(in):: j_sparse(la)
real(kr), intent(in):: a_sparse(la)
integer, intent(in):: la
integer, intent(in):: is_assembled_int
integer, intent(in):: luser_constraints1
integer, intent(in):: luser_constraints2
real(kr), intent(in):: user_constraints(luser_constraints1*&
                                     luser_constraints2)

integer, intent(in):: lelement_data1
integer, intent(in):: lelement_data2
real(kr), intent(in):: element_data(lelement_data1*lelement_data2)
integer, intent(in):: ldof_data
real(kr), intent(in):: dof_data(ldof_data)

```

Description

If distribution of data into subdomains exists already in the user application, data should be loaded into the solver using this routine. It may be called repeatedly by each process if more than one subdomain are assigned to that process. It loads the local mesh of the subdomain and assembled subdomain matrix in the coordinate format. Most data are localized to subdomain.

If partitioning into subdomains does not exist in user's application, routine `bddcml_upload_global_data` should be preferred.

Parameters

<code>nelem</code>	GLOBAL number of elements
<code>nmod</code>	GLOBAL number of nodes
<code>ndof</code>	GLOBAL number of degrees of freedom, i.e. size of matrix
<code>ndim</code>	number of space dimensions
<code>meshdim</code>	mesh dimension. For 3D elements = <code>ndim</code> , for 3D shells = 2, for 3D beams = 1
<code>isub</code>	GLOBAL index of subdomain which is loaded
<code>nelems</code>	LOCAL number of elements in subdomain

<code>nnodes</code>	LOCAL number of nodes in subdomain mesh
<code>ndofs</code>	LOCAL number of degrees of freedom in subdomain mesh
<code>inet</code>	LOCAL array with Indices of Nodes on Elements - this defines connectivity of the subdomain mesh.
<code>linet</code>	length of array <code>inet</code> . It is given as a sum of entries in array <code>nnet</code> .
<code>nnet</code>	LOCAL array with Number of Nodes on Elements. For each element, it gives number of nodes it is connected to. This is important to locate element entries in array <code>inet</code>
<code>lnnet</code>	length of array <code>nnet</code> . It is equal to <code>nelems</code> .
<code>nndf</code>	LOCAL array with Number of Nodal Degrees of Freedom. For each node, it gives number of attached degrees of freedom.
<code>lnndf</code>	length of array <code>nndf</code> . It is equal to <code>nnodes</code> .
<code>isngn</code>	array of Indices of Subdomain Nodes in Global Numbering (local to global map of nodes). For each local node gives the global index in original mesh.
<code>lisngn</code>	length of array <code>isngn</code> . It is equal to <code>nnodes</code> .
<code>isvgvn</code>	array of Indices of Subdomain Variables in Global Variable Numbering (local to global map of variables). For each local degree of freedom gives the global index in original matrix.
<code>lisvgvn</code>	length of array <code>isvgvn</code> . It is equal to <code>ndofs</code> .
<code>isegn</code>	array of Indices of Subdomain Elements in Global Numbering (local to global map of elements). For each subdomain element gives global number in original mesh.
<code>lisegn</code>	length of array <code>isegn</code> . It is equal to <code>nelems</code> .
<code>xyz</code>	LOCAL array with coordinates of nodes as one array (all X, all Y, all Z) or as two-dimensional array in Fortran (X Y Z). Rows are defined by nodes, columns are defined by dimension.
<code>lxyz1,lxyz2</code>	dimensions of array <code>xyz</code> . In C, length of <code>xyz</code> is defined as <code>lxyz1 * lxyz2</code> . In Fortran, dimension of <code>xyz</code> is used as <code>xyz(lxyz1,lxyz2)</code> . The <code>lxyz1</code> is equal to <code>nnodes</code> . The <code>lxyz2</code> is equal to <code>ndim</code> .
<code>ifix</code>	LOCAL array of Indices of FIXED variables - all degrees of freedom with Dirichlet boundary condition are marked by 1, degrees of freedom not prescribed are marked by 0, i.e. non-zero entries determine fixed degrees of freedom. The values of prescribed boundary conditions are given by corresponding entries of array <code>fixv</code> .
<code>lifix</code>	length of array <code>ifix</code> , equal to <code>ndofs</code> .
<code>fixv</code>	LOCAL array of FIXED Variables - where <code>ifix</code> is non-zero, <code>fixv</code> stores value of Dirichlet boundary condition. Where <code>ifix</code> is zero, corresponding value in <code>fixv</code> is meaningless.

<code>lfixv</code>	length of array <code>fixv</code> , equal to <code>ndofs</code> .
<code>rhs</code>	LOCAL array with Right-Hand Side. Values at nodes repeated among subdomains are copied and not weighted.
<code>lrhs</code>	length of array <code>rhs</code> , equal to <code>ndofs</code> .
<code>is_rhs_complete</code>	is the subdomain right-hand side complete? <ul style="list-style-type: none"> • 0 - no, e.g. if only local subassembly of right-hand side was performed - interface values are not fully assembled, solver does not apply weights • 1 - yes, e.g. if local right-hand side is a restriction of the global array to the subdomain - interface values are complete and repeated for more subdomains, solver applies weights to handle multiplicity of these entries
<code>sol</code>	LOCAL array with initial SOLution guess. This is used as initial approximation for iterative method.
<code>lsol</code>	length of array <code>sol</code> , equal to <code>ndofs</code> .
<code>matrixtype</code>	Type of the matrix. This parameter determines storage and underlying direct method of the MUMPS solver for factorizations. Matrix is loaded in coordinate format by three arrays described below. Options are <ul style="list-style-type: none"> • 0 unsymmetric - whole matrix is loaded • 1 symmetric positive definite - only upper triangle of the matrix is loaded • 2 general symmetric - only upper triangle of the matrix is loaded
<code>i_sparse</code>	array of row indices of non-zero entries in LOCAL numbering with respect to subdomain degrees of freedom, i.e. indices are in the range <code>[0, ndofs-1]</code> in C (and in <code>[1, ndofs]</code> in Fortran)
<code>j_sparse</code>	array of column indices of non-zero entries in LOCAL numbering with respect to subdomain degrees of freedom, see <code>i_sparse</code> for their ranges
<code>a_sparse</code>	array of values of non-zero entries
<code>la</code>	length of previous arrays <code>i_sparse</code> , <code>j_sparse</code> , <code>a_sparse</code> (equal to number of non-zeros if the matrix is loaded already assembled)
<code>is_assembled_int</code>	is the matrix assembled? The solver comes with fast assembly routine so the users might want to pass just unassembled matrix for each subdomain (i.e. copy of element matrices equipped with global indexing), and let the solver assemble it. <ul style="list-style-type: none"> • 0 - no, it can contain repeated entries, will be assembled by solver • 1 - yes, it is sorted and does not contain repeated index pairs
<code>luser_constraints1</code> , <code>luser_constraints2</code>	dimension of array with user constraints, <code>luser_constraints2</code> should equal to <code>nnods</code> if user wants to use this feature. Otherwise both can be set to 0.

user_constraints

linearized matrix of user's constraints, one row per constraint, stored row-by-row. Each row has entries for all nodes (in columns) and may contain several constraints (at rows). It may be left empty if no additional constraints are demanded by call to `bddcml_setup_preconditioner`.

lelement_data1, lelement_data2

dimension of array with data for elements, `lelement_data2` should equal to `nelems` if user wants to use this feature. Otherwise both can be set to 0.

element_data

linearized matrix with element data, one row per field, stored row-by-row. Each row has entries for all elements (in columns). Single row is currently optionally used for generating interface weights in the BDDC method, so called ρ -scaling.

ldof_data

dimension of array with data for subdomain degrees of freedom, `ldof_data` should equal to `ndofs` if user wants to use this feature. Otherwise it can be set to 0.

dof_data

coefficients for each local degree of freedom currently optionally used for generating interface weights in the BDDC method. The array should be positive, `dof_data > 0`.

4.4 bddcml_setup_preconditioner

C interface

```
void bddcml_setup_preconditioner( int *matrixtype, int *use_defaults_int,
int *parallel_division_int, int *use_arithmetic_constraints_int, int *use_
adaptive_constraints_int, int *use_user_constraints_int, int *weights_type );
```

Fortran interface

```
subroutine bddcml_setup_preconditioner(matrixtype, use_defaults_int, &
parallel_division_int, & use_arithmetic_constraints_int, & use_adaptive_
constraints_int, & use_user_constraints_int, & weights_type)
```

```
integer,intent(in) :: matrixtype
integer,intent(in) :: use_defaults_int
integer,intent(in) :: parallel_division_int
integer,intent(in) :: use_arithmetic_constraints_int
integer,intent(in) :: use_adaptive_constraints_int
integer,intent(in) :: use_user_constraints_int
integer,intent(in) :: weights_type
```

Description

Calling this function prepares internal data of the preconditioner. Local factorizations are performed for each subdomain at each level and also the resulting coarse problem on the final level is factored. This might be quite costly routine. Once the preconditioner is set-up, it can be reused for new right hand sides (if the matrix is not changed) by calling `bddcml_upload_subdomain_data` followed by `bddcml_solve`.

Parameters

`matrixtype`

Type of the matrix. This parameter determines storage and underlying direct method of the MUMPS solver for factorizations. Should keep the value inserted to `bddcml_upload_subdomain_data`. Options are

- 0 unsymmetric - whole matrix is loaded
- 1 symmetric positive definite - only upper triangle of the matrix is loaded
- 2 general symmetric - only upper triangle of the matrix is loaded

`use_defaults_int`

If > 0 , other options are ignored and the solver uses default options.

`parallel_division_int`

If > 0 , solver will use ParMETIS to create division on first level. This option is only used for global input (`bddcml_upload_global_data`) and only applies to the first level. Otherwise, METIS is used. Default is 1.

`use_arithmetic_constraints_int`

If > 0 , solver will use continuity of arithmetic averages on faces in 2D and faces and edges in 3D to form the coarse space. Default is 1.

use_adaptive_constraints_int

If > 0 , solver will use adaptive averages on faces in 2D and faces in 3D. This might be costly and should be used for very ill-conditioned problems. A generalized eigenvalue problem is solved at each face and weighted averages are derived from eigenvectors. For solving individual eigenproblems, BLOPEX package is used. Default is 0.

use_user_constraints_int

If > 0 , solver will use array `USER_CONSTRAINTS` supplied in routine `bddcml_upload_subdomain_data` for construction of additional constraints on subdomain faces. This may be used e.g. for enforcing flux-based constraints for advection-diffusion problems. Default is 0.

weights_type

Type of weights to be used on interface (default 0). Possible choices

- 0 – weights computed by cardinality, i.e. arithmetic average, the mean value of solution from neighbouring subdomains. Good choice for many problem types except those with large variations in material coefficients and/or sizes of elements.
- 1 – weights from diagonal stiffness, corresponding diagonal entry in the matrix. Good choice for symmetric positive definite problems with large variations in material coefficients and/or sizes of elements. Not good for homogenous problems with irregular subdomains, such as those from graph partitioners, in combination with nodal elements. This option takes into account different sizes of elements and material coefficients.
- 2 – weights based on loaded element data. For this choice, the first row of array `element_data` from function `bddcml_upload_subdomain_data` must contain element coefficients to be used here. This allows definition of the so called ρ -scaling. Good choice for problems with large variations in material coefficients if irregular subdomains from graph partitioners are used in combination with nodal finite elements.
- 3 – weights based on loaded data for degrees of freedom. For this choice, array `dof_data` from function `bddcml_upload_subdomain_data` must contain coefficients for each subdomain degree of freedom. This allows definition of general user-defined weights on degrees of freedom tailored to particular applications.

4.5 bddcml_solve

C interface

```
void bddcml_solve( int *comm_all, int *method, double *tol, int
*maxit, int *ndecrmax, int *recycling_int, int *max_number_of_
stored_vectors, int *num_iter, int *converged_reason, double
*condition_number);
```

Fortran interface

```
subroutine bddcml_solve(comm_all,method,tol,maxit,ndecrmax, &
recycling_int, max_number_of_stored_vectors, & num_iter,converged_
reason,condition_number)
```

```
integer, intent(in) :: comm_all
integer, intent(in) :: method
real(kr), intent(in) :: tol
integer, intent(in) :: maxit
integer, intent(in) :: ndecrmax
integer, intent(in) :: recycling_int
integer, intent(in) :: max_number_of_stored_vectors
integer, intent(out) :: num_iter
integer, intent(out) :: converged_reason
real(kr), intent(out) :: condition_number
```

Description

This function launches the solution procedure for prepared data. System is solved either by preconditioned conjugate gradient (PCG) method or by preconditioned stabilized Bi-Conjugate Gradient (BiCGstab) method.

Parameters

`comm_all` global communicator. Should be the same as `comm_init` for `bddcml_init` function.

`method` Krylov subspace iterative method

- -1 - use defaults - `tol`, `maxit`, and `ndecrmax` not accessed, BiCGstab method used by default,
- 0 - use PCG,
- 1 - use BiCGstab.

`tol` desired accuracy of relative residual (default 1.e-6).

`maxit` limit on number of iterations (default 1000).

`ndecrmax` limit on number of iterations with non-decreasing residual (default 30) - used to stop a diverging process.

`recycling_int`

If > 0 , the Krylov subspace will be recycled in the Krylov subspace method (default 0). This can save time for solutions for many

right-hand sides. The option triggers explicit orthogonalization to the stored Krylov basis. Therefore, even if this option is used with just one right-hand side solve, it can help the convergence for numerically complicated problems, where natural orthogonality of the basis may be lost. The approach to recycling is based on Farhat, C., Crivelli, L., Roux, X.: Extending substructure based iterative solvers to multiple load and repeated analyses. *Comput. Methods in Appl. Mech. Engrg.* 117 (1994), 195-209.

max_number_of_stored_vectors

limit on the size of the Krylov subspace basis explicitly kept in the solver (default 100). Only meaningful if `recycling_int > 0`.

num_iter on output, resulting number of iterations.

converged_reason

on output, contains reason for convergence/divergence

- 0 - converged relative residual,
- -1 - reached limit on number of iterations,
- -2 - reached limit on number of iterations with non-decreasing residual.

condition_number

on output, estimated condition number (for PCG only).

4.6 bddcml_download_local_solution

C interface

```
void bddcml_download_local_solution( int *isub, double *sols, int
*lsols );
```

Fortran interface

```
subroutine bddcml_download_local_solution(isub, sols,lsols)
    integer, intent(in):: isub
    integer, intent(in):: lsols
    real(kr), intent(out):: sols(lsols)
```

Description

Subroutine for getting local solution, i.e. restriction of solution vector to subdomain (no weights are applied).

Parameters

<code>isub</code>	GLOBAL index of subdomain
<code>sols</code>	LOCAL array of solution restricted to subdomain
<code>lsols</code>	length of array <code>sols</code> , equal to <code>ndofs</code> .

4.7 bddcml_download_global_solution

C interface

```
void bddcml_download_global_solution( double *sol, int *lsol );
```

Fortran interface

```
subroutine bddcml_download_global_solution(sol, lsol)
    integer, intent(in):: lsol
    real(kr), intent(out):: sol(lsol)
```

Description

This function downloads global solution of the system from the solver at the root process.

Parameters

<code>sol</code>	GLOBAL array of solution
<code>lsol</code>	length of array <code>sol</code> , equal to <code>ndof</code>

4.8 bddcml_download_local_reactions

C interface

```
void bddcml_download_local_reactions( int *isub, double *reas, int
*lreas );
```

Fortran interface

```
subroutine bddcml_download_local_reactions(isub, reas,lreas)
    integer, intent(in):: isub
    integer, intent(in):: lreas
    real(kr), intent(out):: reas(lreas)
```

Description

Subroutine for getting local reactions at unknowns fixed by Dirichlet boundary conditions, i.e. restriction of vector of reactions to subdomain (no weights are applied). Global vector of reactions is given by $\mathbf{r} = \mathbf{Ax} - \mathbf{b}$, where \mathbf{A} is the matrix WITHOUT Dirichlet boundary conditions fixed, \mathbf{x} is the solution, and \mathbf{b} the original right-hand side.

Parameters

<code>isub</code>	GLOBAL index of subdomain
<code>reas</code>	LOCAL array of vector of reactions restricted to subdomain. It contains nonzeros only at unknowns marked in the IFIX array (see <code>bddcml_upload_local_data</code>).
<code>lreas</code>	length of array <code>reas</code> , equal to <code>ndofs</code> .

4.9 bddcml_download_global_reactions

C interface

```
void bddcml_download_global_reactions( double *rea, int *lrea );
```

Fortran interface

```
subroutine bddcml_download_global_reactions(rea, lrea)
    integer, intent(in):: lrea
    real(kr), intent(out):: rea(lrea)
```

Description

Subroutine for getting global reactions at unknowns fixed by Dirichlet boundary conditions at the root process. Global vector of reactions is given by $\mathbf{r} = \mathbf{Ax} - \mathbf{b}$, where \mathbf{A} is the matrix WITHOUT Dirichlet boundary conditions fixed, \mathbf{x} is the solution, and \mathbf{b} the original right-hand side.

Parameters

rea GLOBAL array of reactions. It contains nonzeros only at unknowns marked in the IFIX array (see `bddcml_upload_global_data`).

lrea length of array `rea`, equal to `ndof`

4.10 bddcml_change_global_data

C interface

```
void bddcml_change_global_data( int *ifix, int *lifix, double
*fixv, int *lfixv, double *rhs, int *lrhs, double *sol, int *lsol);
```

Fortran interface

```
subroutine bddcml_change_global_data(ifix,lifix, fixv,lfixv,
rhs,lrhs, sol,lsol)
    integer, intent(in):: lifix
    integer, intent(in):: ifix(lifix)
    integer, intent(in):: lfixv
    real(kr), intent(in):: fixv(lfixv)
    integer, intent(in):: lrhs
    real(kr), intent(in):: rhs(lrhs)
    integer, intent(in):: lsol
    real(kr), intent(in):: sol(lsol)
```

Description

A function for loading another right hand side, when global loading is used. Position of fixed variables, the IFIX array, is not allowed to change. Parameters correspond to routine `bddcml_upload_global_data`.

Parameters

<code>ifix</code>	GLOBAL array of Indices of FIXed variables - all degrees of freedom with Dirichlet boundary condition are marked by 1, degrees of freedom not prescribed are marked by 0, i.e. non-zero entries determine fixed degrees of freedom. The values of prescribed boundary conditions are given by corresponding entries of array <code>fixv</code> .
<code>lifix</code>	length of array <code>ifix</code> , equal to <code>ndof</code> .
<code>fixv</code>	GLOBAL array of FIXed Variables - where <code>ifix</code> is non-zero, <code>fixv</code> stores value of Dirichlet boundary condition. Where <code>ifix</code> is zero, corresponding value in <code>fixv</code> is meaningless.
<code>lfixv</code>	length of array <code>fixv</code> , equal to <code>ndof</code> .
<code>rhs</code>	GLOBAL array with Right-Hand Side
<code>lrhs</code>	length of array <code>rhs</code> , equal to <code>ndof</code> .
<code>sol</code>	GLOBAL array with initial SOLution guess. This is used as initial approximation for iterative method.
<code>lsol</code>	length of array <code>sol</code> , equal to <code>ndof</code> .

4.11 bddcml_change_subdomain_data

C interface

```
void bddcml_change_subdomain_data( int *isub, int *ifix, int
*lifix, double *fixv, int *lfixv, double *rhs, int *lrhs, int
*is_rhs_complete, double *sol, int *lsol );
```

Fortran interface

```
subroutine bddcml_change_subdomain_data(isub, & ifix,lifix,
fixv,lfixv, & rhs,lrhs, is_rhs_complete_int, & sol,lsol)
    integer, intent(in):: isub
    integer, intent(in):: lifix
    integer, intent(in):: ifix(lifix)
    integer, intent(in):: lfixv
    real(kr), intent(in):: fixv(lfixv)
    integer, intent(in):: lrhs
    real(kr), intent(in):: rhs(lrhs)
    integer, intent(in):: is_rhs_complete_int
    integer, intent(in):: lsol
    real(kr), intent(in):: sol(lsol)
```

Description

A function for loading another right hand side, when subdomain-by-subdomain loading is used. Position of fixed variables, the `IFIX` array, is not allowed to change. Parameters correspond to routine `bddcml_upload_subdomain_data`. It should be called repeatedly by each process if more than one subdomain are assigned to that process. This call should be followed by calling `bddcml_setup_new_data` before another call to `bddcml_solve`.

If partitioning into subdomains does not exist in user's application, routine `bddcml_change_global_data` should be preferred.

Parameters

<code>isub</code>	GLOBAL index of subdomain which is loaded
<code>ifix</code>	LOCAL array of Indices of FIXed variables - all degrees of freedom with Dirichlet boundary condition are marked by 1, degrees of freedom not prescribed are marked by 0, i.e. non-zero entries determine fixed degrees of freedom. The values of prescribed boundary conditions are given by corresponding entries of array <code>fixv</code> .
<code>lifix</code>	length of array <code>ifix</code> , equal to <code>ndofs</code> .
<code>fixv</code>	LOCAL array of FIXed Variables - where <code>ifix</code> is non-zero, <code>fixv</code> stores value of Dirichlet boundary condition. Where <code>ifix</code> is zero, corresponding value in <code>fixv</code> is meaningless.
<code>lfixv</code>	length of array <code>fixv</code> , equal to <code>ndofs</code> .

<code>rhs</code>	LOCAL array with Right-Hand Side. Values at nodes repeated among subdomains are copied and not weighted.
<code>lrhs</code>	length of array <code>rhs</code> , equal to <code>ndofs</code> .
<code>is_rhs_complete</code>	is the subdomain right-hand side complete? <ul style="list-style-type: none">• 0 - no, e.g. if only local subassembly of right-hand side was performed - interface values are not fully assembled, solver does not apply weights• 1 - yes, e.g. if local right-hand side is a restriction of the global array to the subdomain - interface values are complete and repeated for more subdomains, solver applies weights to handle multiplicity of these entries
<code>sol</code>	LOCAL array with initial SOLUTION guess. This is used as initial approximation for iterative method.
<code>lsol</code>	length of array <code>sol</code> , equal to <code>ndofs</code> .

4.12 bddcml_setup_new_data

C interface

```
void bddcml_setup_new_data( );
```

Fortran interface

```
subroutine bddcml_setup_new_data
```

Description

Setting up internal data-structures for handling new values of Dirichlet boundary conditions and right hand side — creating new reduced right-hand side.

Needs to be called after calling `bddcml_change_subdomain_data` or `bddcml_change_global_data` and before another call to `bddcml_solve`.

Parameters

This routine currently does not take any arguments.

4.13 bddcml_dotprod_subdomain

C interface

```
void bddcml_dotprod_subdomain( int *isub, double *vec1, int *lvec1,
double *vec2, int *lvec2, double *dotprod );
```

Fortran interface

```
subroutine bddcml_dotprod_subdomain( isub, vec1,lvec1, vec2,lvec2,
dotprod )
```

```
integer, intent(in) :: isub
integer, intent(in) :: lvec1
real(kr), intent(in) :: vec1(lvec1)
integer, intent(in) :: lvec2
real(kr), intent(in) :: vec2(lvec2)
real(kr), intent(out) :: dotprod
```

Description

Auxiliary subroutine to compute scalar product of two vectors of length of subdomain exploiting interface weights from the solver. This routine is useful if we want to compute global norm or dot-product based on vectors restricted to subdomains. Since interface values are contained in several vectors for several subdomains, this dot product or norm cannot be determined without weights.

Parameters

<code>isub</code>	GLOBAL index of subdomain
<code>vec1</code>	LOCAL first vector for dot-product
<code>lvec1</code>	length of <code>vec1</code>
<code>vec2</code>	LOCAL second vector for dot-product, may be same array as <code>vec1</code>
<code>lvec2</code>	length of <code>vec2</code> , should be same as <code>lvec1</code>
<code>dotprod</code>	on exit, returns <code>vec1' * weights * vec2</code>

4.14 bddcml_finalize

C interface

```
void bddcml_finalize( );
```

Fortran interface

```
subroutine bddcml_finalize
```

Description

Finalization of the solver. All internal data are deallocated.

Parameters

This routine currently does not take any arguments.