User Documentation for IDA v2.5.0

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Chapter 1

Introduction

IDA is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [12]. This suite consists of CVODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities.

IDA is a general purpose solver for the initial value problem for systems of differential-algebraic equations (DAEs). The name IDA stands for Implicit Differential-Algebraic solver. IDA is based on DASPK [3, 4], but is written in ANSI-standard C rather than FORTRAN77. Its most notable feature is that, in the solution of the underlying nonlinear system at each time step, it offers a choice of Newton/direct methods and a choice of Inexact Newton/Krylov (iterative) methods. Thus IDA shares significant modules previously written within CASC at LLNL to support the ordinary differential equation (ODE) solvers CVODE [14, 8] and PVODE [6, 7], and also the nonlinear system solver KINSOL [9].

The Newton/Krylov methods in IDA are: the GMRES (Generalized Minimal RESidual) [16], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [17], and TFQMR (Transpose-Free Quasi-Minimal Residual) linear iterative methods [10]. As Krylov methods, these require almost no matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner matrix, and for most problems preconditioning is essential for an efficient solution.

For very large DAE systems, the Krylov methods are preferable over direct linear solver methods, and are often the only feasible choice. Among the three Krylov methods in IDA, we recommend GMRES as the best overall choice. However, users are encouraged to compare all three, especially if encountering convergence failures with GMRES. Bi-CGFStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size.

There are several motivations for choosing the C language for IDA. First, a general movement away from FORTRAN and toward C in scientific computing is apparent. Second, the pointer, structure, and dynamic memory allocation features in C are extremely useful in software of this complexity, with the great variety of method options offered. Finally, we prefer C over C++ for IDA because of the wider availability of C compilers, the potentially greater efficiency of C, and the greater ease of interfacing the solver to applications written in extended FORTRAN.

1.1 Changes from previous versions

Changes in v2.5.0

The main changes in this release involve a rearrangement of the entire SUNDIALS source tree (see §4.1). At the user interface level, the main impact is in the mechanism of including SUNDIALS header files which must now include the relative path (e.g. `#include <cvode/cvode.h>`). Additional changes were made to the build system: all exported header files are now installed in separate subdirectories of the instaltion *include* directory.

A bug was fixed in the internal difference-quotient dense and banded Jacobian approximations, related to the estimation of the perturbation (which could have lead to a failure of the linear solver when zero components with sufficiently small absolute tolerances were present).

The user interface to the consistent initial conditions calculations has been modified. The `IDACalcIC` arguments `t0`, `yy0`, and `yp0` were removed and a new function, `IDAGetconsistentIC` is provided (see §5.5.4 and §5.5.8.2 for details).

The functions in the generic dense linear solver (`sundials_dense` and `sundials_smalldense`) were modified to work for rectangular $m \times n$ matrices ($m \leq n$), while the factorization and solution functions were renamed to `DenseGETRF`/`denGETRF` and `DenseGETRS`/`denGETRS`, respectively. The factorization and solution functions in the generic band linear solver were renamed `BandGBTRF` and `BandGBTRS`, respectively.

Changes in v2.4.0

FIDA, a FORTRAN-C interface module, was added (for details see Chapter 6).

IDASPBCG and IDASPTFQMR modules have been added to interface with the Scaled Preconditioned Bi-CGstab (SPBCG) and Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR) linear solver modules, respectively (for details see Chapter 5). At the same time, function type names for Scaled Preconditioned Iterative Linear Solvers were added for the user-supplied Jacobian-times-vector and preconditioner setup and solve functions.

The rootfinding feature was added, whereby the roots of a set of given functions may be computed during the integration of the DAE system.

A user-callable routine was added to access the estimated local error vector.

The deallocation functions now take as arguments the address of the respective memory block pointer.

To reduce the possibility of conflicts, the names of all header files have been changed by adding unique prefixes (`ida_` and `sundials_`). When using the default installation procedure, the header files are exported under various subdirectories of the target `include` directory. For more details see §2.

Changes in v2.3.0

The user interface has been further refined. Several functions used for setting optional inputs were combined into a single one. An optional user-supplied routine for setting the error weight vector was added. Additionally, to resolve potential variable scope issues, all SUNDIALS solvers release user data right after its use. The build systems has been further improved to make it more robust.

Changes in v2.2.2

Minor corrections and improvements were made to the build system. A new chapter in the User Guide was added — with constants that appear in the user interface.

Changes in v2.2.1

The changes in this minor SUNDIALS release affect only the build system.

Changes in v2.2.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the `iopt` and `ropt` arrays. Instead, IDA now provides a set of routines (with prefix `IDASet`) to change the default values for various quantities controlling the solver and a set of extraction routines (with prefix `IDAGet`) to extract statistics after return from the main solver routine. Similarly, each linear solver module provides its own set of `Set`- and `Get`-type routines. For more details see §5.5.6 and §5.5.8.

Additionally, the interfaces to several user-supplied routines (such as those providing Jacobians and preconditioner information) were simplified by reducing the number of arguments. The same information that was previously accessible through such arguments can now be obtained through `Get`-type functions.

Installation of IDA (and all of SUNDIALS) has been completely redesigned and is now based on configure scripts.

1.2 Reading this User Guide

The structure of this document is as follows:

- In Chapter 2 we begin with instructions for the installation of IDA, within the structure of SUNDIALS.
- In Chapter 3, we give short descriptions of the numerical methods implemented by IDA for the solution of initial value problems for systems of DAEs.
- The following chapter describes the structure of the SUNDIALS suite of solvers (§4.1) and the software organization of the IDA solver (§4.2).
- Chapter 5 is the main usage document for IDA for C applications. It includes a complete description of the user interface for the integration of DAE initial value problems.
- In Chapter 6, we describe FIDA, an interface module for the use of IDA with FORTRAN applications.
- Chapter 7 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, as well as details on the two NVECTOR implementations provided with SUNDIALS: a serial implementation (§7.1) and a parallel MPI implementation (§7.2).
- Chapter 8 describes the interfaces to the linear solver modules, so that a user can provide his/her own such module.
- Chapter 9 describes in detail the generic linear solvers shared by all SUNDIALS solvers.
- Finally, Chapter 10 lists the constants used for input to and output from IDA.

Finally, the reader should be aware of the following notational conventions in this user guide: program listings and identifiers (such as `IDAMalloc`) within textual explanations appear in typewriter type style; fields in C structures (such as *content*) appear in italics; and packages or modules, such as IDADENSE, are written in all capitals. In the Index, page numbers that appear in bold indicate the main reference for that entry.

Acknowledgments. We wish to acknowledge the contributions to previous versions of the IDA code and user guide of Allan G. Taylor.

Chapter 2

IDA Installation Procedure

The installation of IDA is accomplished by installing the SUNDIALS suite as a whole, according to the instructions that follow. The same procedure applies whether or not the downloaded file contains solvers other than IDA.[1]

The SUNDIALS suite (or individual solvers) are distributed as compressed archives (`.tgz`). The name of the distribution archive is of the form *solver*`-x.y.z.tgz`, where *solver* is one of: `sundials`, `cvode`, `cvodes`, `ida`, or `kinsol`, and `x.y.z` represents the version number (of the SUNDIALS suite or of the individual solver).

To begin the installation, first uncompress and expand the sources, by issuing

```
% tar xzf solver-x.y.z.tgz
```

This will extract source files under a directory *solver*`-x.y.z`.

The installation procedure outlined below will work on commodity LINUX/UNIX systems without modification. However, users are still encouraged to carefully read the entire chapter before attempting to install the SUNDIALS suite, in case non-default choices are desired for compilers, compilation options, or the like. In lieu of reading the option list below, the user may invoke the configuration script with the help flag to view a complete listing of available options, which may be done by issuing

```
% ./configure --help
```

from within the directory created above.

In the remainder of this chapter, we make the following distinctions:

- *srcdir*

  is the directory *solver*`-x.y.z` created above; i.e., the directory containing the SUNDIALS sources.

- *builddir*

  is the directory under which SUNDIALS is built; i.e., the directory from within which the `configure` command is issued. Usually, this is the same as *srcdir*.

- *instdir*

  is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory *instdir*`/include` while libraries are installed under *instdir*`/lib`, with *instdir* specified with the `--prefix` flag to `configure`. See §2.1 for more details on the installation directories, including the special cases of the SUNDIALS examples and the SUNDIALSTB toolbox.

Note: The installation directory *instdir* should *not* be the same as the source directory *srcdir*.

[1] Files for both the serial and parallel versions of IDA are included in the distribution. For users in a serial computing environment, the files specific to parallel environments (which may be deleted) are as follows: all files in `src/nvec_par/`; `ida_bbdpre.c, ida_bbdpre_impl.h` (in `src/ida/`); `ida_bbdpre.h` (in `include/ida/`); `fidabbd.c, fidabbd.h` (in `src/ida/fcmix/`); all files in `examples/ida/parallel/`; all files in `examples/ida/fcmix_parallel/`. (By "serial version" of IDA we mean the IDA solver with the serial NVECTOR module attached, and similarly for "parallel version".)

The installation steps for SUNDIALS can be as simple as

```
% tar xzf solver-x.y.z.tgz
% cd solver-x.y.z
% ./configure
% make
% make install
```

in which case the SUNDIALS header files and libraries are installed under `/usr/local/include` and `/usr/local/lib`, respectively. Note that, by default, neither the example programs nor the SUNDIALSTB toolbox are built and installed.

If disk space is a priority, then to delete all temporary files created by building SUNDIALS, issue

```
% make clean
```

To prepare the SUNDIALS distribution for a new install (using, for example, different options and/or installation destinations), issue

```
% make distclean
```

2.1 Configuration options

The installation procedure given above will generally work without modification; however, if the system includes multiple MPI implementations, then certain configure script-related options may be used to indicate which MPI implementation should be used. Also, if the user wants to use non-default language compilers, then, again, the necessary shell environment variables must be appropriately redefined. The remainder of this section provides explanations of available configure script options.

General options

`--prefix=PREFIX`

Location for architecture-independent files.

Default: `PREFIX=`/usr/local

`--exec-prefix=EPREFIX`

Location for architecture-dependent files.

Default: `EPREFIX=`/usr/local

`--includedir=DIR`

Alternate location for installation of header files.

Default: `DIR=PREFIX/include`

`--libdir=DIR`

Alternate location for installation of libraries.

Default: `DIR=EPREFIX/lib`

`--disable-`*solver*

Although each existing solver module is built by default, support for a given solver can be explicitly disabled using this option. The valid values for *solver* are: `cvode`, `cvodes`, `ida`, and `kinsol`.

`--enable-examples`

Available example programs are *not* built by default. Use this option to enable compilation of all pertinent example programs. Upon completion of the `make` command, the example executables will be created under solver-specific subdirectories of *builddir*`/examples`:

builddir/examples/*solver*/serial : serial C examples

builddir/examples/*solver*/parallel : parallel C examples

builddir/examples/*solver*/fcmix_serial : serial FORTRAN examples

builddir/examples/*solver*/fcmix_parallel : parallel FORTRAN examples

Note: Some of these subdirectories may not exist depending upon the solver and/or the configuration options given.

`--with-examples-instdir=EXINSTDIR`

Alternate location for example executables and sample output files (valid only if examples are enabled). Note that installtion of example files can be completely disabled by issuing `EXINSTDIR=no` (in case building the examples is desired only as a test of the SUNDIALS libraries).

Default: `DIR=EPREFIX/examples`

`--with-cppflags=ARG`

Specify additional C preprocessor flags (e.g., `ARG=-I<include_dir>` if necessary header files are located in nonstandard locations).

`--with-cflags=ARG`

Specify additional C compilation flags.

`--with-ldflags=ARG`

Specify additional linker flags (e.g., `ARG=-L<lib_dir>` if required libraries are located in nonstandard locations).

`--with-libs=ARG`

Specify additional libraries to be used (e.g., `ARG=-l<foo>` to link with the library named `libfoo.a` or `libfoo.so`).

`--with-precision=ARG`

By default, SUNDIALS will define a real number (internally referred to as `realtype`) to be a double-precision floating-point numeric data type (`double` C-type); however, this option may be used to build SUNDIALS with `realtype` alternatively defined as a single-precision floating-point numeric data type (`float` C-type) if `ARG=single`, or as a `long double` C-type if `ARG=extended`.

Default: `ARG=double`

Users should *not* build SUNDIALS with support for single-precision floating-point arithmetic on 32- or 64-bit systems. This will almost certainly result in unreliable numerical solutions. The configuration option `--with-precision=single` is intended for systems on which single-precision arithmetic involves at least 14 decimal digits.

Options for Fortran support

`--disable-fcmix`

Using this option will disable all FORTRAN support. The FCVODE, FKINSOL, FIDA, and FNVECTOR modules will not be built, regardless of availability.

`--with-fflags=ARG`

Specify additional FORTRAN compilation flags.

The configuration script will attempt to automatically determine the function name mangling scheme required by the specified FORTRAN compiler, but the following two options may be used to override the default behavior.

`--with-f77underscore=ARG`

This option pertains to the FCVODE, FKINSOL, FIDA, and FNVECTOR FORTRAN-C interface modules and is used to specify the number of underscores to append to function names so FORTRAN routines can properly link with the associated SUNDIALS libraries. Valid values for `ARG` are: `none`, `one` and `two`.

Default: `ARG=one`

`--with-f77case=ARG`

Use this option to specify whether the external names of the FCVODE, FKINSOL, FIDA, and FNVECTOR FORTRAN-C interface functions should be lowercase or uppercase so FORTRAN routines can properly link with the associated SUNDIALS libraries. Valid values for `ARG` are: `lower` and `upper`.

Default: `ARG=lower`

Options for MPI support

The following configuration options are only applicable to the parallel SUNDIALS packages:

`--disable-mpi`

Using this option will completely disable MPI support.

`--with-mpicc=ARG`

`--with-mpif77=ARG`

By default, the configuration utility script will use the MPI compiler scripts named `mpicc` and `mpif77` to compile the parallelized SUNDIALS subroutines; however, for reasons of compatibility, different executable names may be specified via the above options. Also, `ARG=no` can be used to disable the use of MPI compiler scripts, thus causing the serial C and FORTRAN compilers to be used to compile the parallelized SUNDIALS functions and examples.

`--with-mpi-root=MPIDIR`

This option may be used to specify which MPI implementation should be used. The SUNDIALS configuration script will automatically check under the subdirectories `MPIDIR/include` and `MPIDIR/lib` for the necessary header files and libraries. The subdirectory `MPIDIR/bin` will also be searched for the C and FORTRAN MPI compiler scripts, unless the user uses `--with-mpicc=no` or `--with-mpif77=no`.

`--with-mpi-incdir=INCDIR`

`--with-mpi-libdir=LIBDIR`

`--with-mpi-libs=LIBS`

These options may be used if the user would prefer not to use a preexisting MPI compiler script, but instead would rather use a serial complier and provide the flags necessary to compile the MPI-aware subroutines in SUNDIALS.

Often an MPI implementation will have unique library names and so it may be necessary to specify the appropriate libraries to use (e.g., `LIBS=-lmpich`).

Default: `INCDIR=MPIDIR/include` and `LIBDIR=MPIDIR/lib`

`--with-mpi-flags=ARG`

Specify additional MPI-specific flags.

Options for library support

By default, only static libraries are built, but the following option may be used to build shared libraries on supported platforms.

`--enable-shared`

Using this particular option will result in both static and shared versions of the available SUNDIALS libraries being built if the system supports shared libraries. To build only shared libraries also specify `--disable-static`.

Note: The FCVODE, FKINSOL, and FIDA libraries can only be built as static libraries because they contain references to externally defined symbols, namely user-supplied FORTRAN subroutines. Although the FORTRAN interfaces to the serial and parallel implementations of the supplied NVECTOR module do not contain any unresolvable external symbols, the libraries are still built as static libraries for the purpose of consistency.

Options for Matlab support

The following options are relevant only for configuring and building the SUNDIALSTB Matlab toolbox:

`--enable-sundialsTB`

The SUNDIALSTB Matlab toolbox is *not* built by default. Use this option to enable configuration and compilation of the `mex` files. Upon completion of the `make` command, the following `mex` files will be created:

builddir`/sundialsTB/cvodes/cvm/cvm.`*mexext*

builddir`/sundialsTB/idas/idm/idm.`*mexext*

builddir`/sundialsTB/kinsol/kim/kim.`*mexext*

where *mexext* is the platform-specific extension of `mex` files.

`--with-sundialsTB-instdir=STBINSTDIR`

Alternate location for the installed SUNDIALSTB toolbox (valid only if SUNDIALSTB is enabled). As for the example programs, installation of SUNDIALSTB can be completely disabled by issuing `STBINSTDIR=no` (in case building the toolbox is desired but its installtion will be done manually afterwards). Otherwise, all required SUNDIALSTB files will be installed under the directory `STBINSTDIR/sundialsTB`.

Default: `DIR=MATLAB/toolbox` (see below for the definition of `MATLAB`).

`--with-matlab=MATLAB`

This option can be used to specify the location of the Matlab executable. The default is to search the path.

`--with-mexopts=ARG`

Specify the `mex` options file to be used.

Default: Standard Matlab `mex` options file.

`--with-mexflags=ARG`

Specify the `mex` compiler flags to be used.

Default: `ARG=-O`

`--with-mexldadd=ARG`

Specify additional `mex` linker flags.

Default: none

Environment variables

The following environment variables can be locally (re)defined for use during the configuration of SUNDIALS. See the next section for illustrations of these.

`CC`

`F77`

Since the configuration script uses the first C and FORTRAN compilers found in the current executable search path, then each relevant shell variable (`CC` and `F77`) must be locally (re)defined in order to use a different compiler. For example, to use `xcc` (executable name of chosen compiler) as the C language compiler, use `CC=xcc` in the configure step.

`CFLAGS`

`FFLAGS`

Use these environment variables to override the default C and FORTRAN compilation flags.

2.2 Configuration examples

The following examples are meant to help demonstrate proper usage of the configure options.

To build SUNDIALS using the default C and Fortran compilers, and default `mpicc` and `mpif77` parallel compilers, enable compilation of examples, build the Matlab `mex` files for SUNDIALSTB, and install it under `/home/myname/matlab/sundialsTB`, use

```
% configure --prefix=/home/myname/sundials --enable-examples \
            --enable-sundialsTB --with-sundialsTB-instdir=/home/myname/matlab
```

To disable installation of the examples, use:

```
% configure --prefix=/home/myname/sundials \
            --enable-examples --with-examples-instdir=no \
            --enable-sundialsTB --with-sundialsTB-instdir=/home/myname/matlab
```

The following example builds SUNDIALS using `gcc` as the serial C compiler, `g77` as the serial FORTRAN compiler, `mpicc` as the parallel C compiler, `mpif77` as the parallel FORTRAN compiler, and appends the `-g3` compilaton flag to the list of default flags:

```
% configure CC=gcc F77=g77 --with-cflags=-g3 --with-fflags=-g3 \
            --with-mpicc=/usr/apps/mpich/1.2.4/bin/mpicc \
            --with-mpif77=/usr/apps/mpich/1.2.4/bin/mpif77
```

The next example again builds SUNDIALS using `gcc` as the serial C compiler, but the `--with-mpicc=no` option explicitly disables the use of the corresponding MPI compiler script. In addition, since the `--with-mpi-root` option is given, the compilation flags `-I/usr/apps/mpich/1.2.4/include` and `-L/usr/apps/mpich/1.2.4/lib` are passed to `gcc` when compiling the MPI-enabled functions. The `--disable-examples` option explicitly disables the examples (which means a FORTRAN compiler is not required). The `--with-mpi-libs` option is required so that the configure script can check if `gcc` can link with the appropriate MPI library.

```
% configure CC=gcc --disable-examples --with-mpicc=no \
            --with-mpi-root=/usr/apps/mpich/1.2.4 \
            --with-mpi-libs=-lmpich
```

2.3 Installed libraries and exported header files

Using the standard SUNDIALS build system, the command

```
% make install
```

will install the libraries under *libdir* and the public header files under *includedir*. The default values for these directories are *instdir*/`lib` and *instdir*/`include`, respectively, but can be changed using the configure script options `--prefix`, `--exec-prefix`, `--includedir` and `--libdir` (see §2.1). For example, a global installation of SUNDIALS on a *NIX system could be accomplished using

```
% configure --prefix=/opt/sundials-2.1.1
```

Although all installed libraries reside under *libdir*, the public header files are further organized into subdirectories under *includedir*.

The installed libraries and exported header files are listed for reference in Table 2.1. The file extension *.lib* is typically `.so` for shared libraries and `.a` for static libraries (see *Options for library support* for additional details).

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the *includedir*/`sundials` directory since they are explicitly included by the appropriate solver header files (*e.g.*, `cvode_dense.h` includes `sundials_dense.h`). However, it is both legal and safe to do so (*e.g.*, the functions declared in `sundials_smalldense.h` could be used in building a preconditioner).

2.4 Building SUNDIALS without the configure script

If the `configure` script cannot be used (*e.g.*, when building SUNDIALS under Microsoft Windows without using Cygwin), or if the user prefers to own the build process (*e.g.*, when SUNDIALS is incorporated into a larger project with its own build system), then the header and source files for a given module can be copied from the *srcdir* to some other location and compiled separately.

The following files are required to compile a SUNDIALS solver module:

- public header files located under *srcdir*/`include/`*solver*
- implementation header files and source files located under *srcdir*/`src/`*solver*
- (optional) FORTRAN/C interface files located under *srcdir*/`src/`*solver*/`fcmix`
- shared public header files located under *srcdir*/`include/sundials`
- shared source files located under *srcdir*/`src/sundials`
- (optional) NVECTOR_SERIAL header and source files located under *srcdir*/`include/nvector` and *srcdir*/`src/nvec_ser`
- (optional) NVECTOR_PARALLEL header and source files located under *srcdir*/`include/nvector` and *srcdir*/`src/nvec_par`
- configuration header file `sundials_config.h` (see below)

A sample header file that, appropriately modified, can be used as `sundials_config.h` (otherwise created automatically by the `configure` script) is provided below. The various preprocessor macros defined within `sundials_config.h` have the following uses:

- Precision of the SUNDIALS `realtype` type

  Only one of the macros `SUNDIALS_SINGLE_PRECISION`, `SUNDIALS_DOUBLE_PRECISION` and `SUNDIALS_EXTENDED_PRECISION` should be defined to indicate if the SUNDIALS `realtype` type is an alias for `float`, `double`, or `long double`, respectively.

Table 2.1: SUNDIALS libraries and header files (names are relative to *libdir* for libraries and to *includedir* for header files)

SHARED	Libraries	n/a	
	Header files	sundials/sundials_types.h	sundials/sundials_math.h
		sundials/sundials_config.h	sundias/sundials_nvector.h
		sundials/sunials_smalldense.h	sundials/sundials_dense.h
		sundials/sundials_iterative.h	sundials/sundials_band.h
		sundials/sundials_spbcgs.h	sundials/sundials_sptfqmr.h
		sundials/sundials_spgmr.h	
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib*	libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h	
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib*	libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h	
CVODE	Libraries	libsundials_cvode.*lib*	libsundials_fcvode.a
	Header files	cvode/cvode.h	
		cvode/cvode_dense.h	cvode/cvode_band.h
		cvode/cvode_diag.h	cvode/cvode_spils.h
		cvode/cvode_bandpre.h	cvode/cvode_bbdpre.h
		cvode/cvode_spgmr.h	cvode/cvode_spbcgs.h
		cvode/cvode_sptfqmr.h	cvode/cvode_impl.h
CVODES	Libraries	libsundials_cvodes.*lib*	
	Header files	cvodes/cvodes.h	
		cvodes/cvodes_dense.h	cvodes/cvodes_band.h
		cvodes/cvodes_diag.h	cvodes/cvodes_spils.h
		cvodes/cvodes_bandpre.h	cvodes/cvodes_bbdpre.h
		cvodes/cvodes_spgmr.h	cvodes/cvodes_spbcgs.h
		cvodes/cvodes_sptfqmr.h	cvodes/cvodes_impl.h
		cvodes/cvodea_impl.h	
IDA	Libraries	libsundials_ida.*lib*	libsundials_fida.a
	Header files	ida/ida.h	
		ida/ida_dense.h	ida/ida_band.h
		ida/ida_spils.h	ida/ida_spgmr.h
		ida/ida_spbcgs.h	ida/ida_sptfqmr.h
		ida/ida_bbdpre.h	ida/ida_impl.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a
	Header files	kinsol/kinsol.h	
		kinsol/kinsol_dense.h	kinsol/kinsol_band.h
		kinsol/kinsol_spils.h	kinsol/kinsol_spgmr.h
		kinsol/kinsol_spbcgs.h	kinsol/kinsol_sptfqmr.h
		kinsol/kinsol_bbdpre.h	kinsol/kinsol_impl.h

- Use of generic math functions

  If SUNDIALS_USE_GENERIC_MATH is defined, then the functions in sundials_math.(h,c) will use the pow, sqrt, fabs, and exp functions from the standard math library (see math.h), regardless of the definition of realtype. Otherwise, if realtype is defined to be an alias for the float C-type, then SUNDIALS will use powf, sqrtf, fabsf, and expf. If realtype is instead defined to be a synonym for the long double C-type, then powl, sqrtl, fabsl, and expl will be used.

  Note: Although the powf/powl, sqrtf/sqrtl, fabsf/fabsl, and expf/expl routines are not specified in the ANSI C standard, they are ISO C99 requirements. Consequently, these routines will only be used if available.

- FORTRAN name-mangling scheme

  The macros given below are used to transform the C-language function names defined in the FORTRAN-C inteface modules in a manner consistent with the preferred FORTRAN compiler, thus allowing native C functions to be called from within a FORTRAN subroutine. The name-mangling scheme can be specified either by appropriately defining the parameterized macros (using the stringization operator, ##, if necessary)

  - F77_FUNC(name,NAME)
  - F77_FUNC_(name,NAME)

  or by defining *one* macro from each of the following lists:

  - SUNDIALS_CASE_LOWER or SUNDIALS_CASE_UPPER
  - SUNDIALS_UNDERSCORE_NONE, SUNDIALS_UNDERSCORE_ONE, or SUNDIALS_UNDERSCORE_TWO

  For example, to specify that mangled C-language function names should be lowercase with one underscore appended include either

  ```
  #define F77_FUNC(name,NAME) name ## _
  #define F77_FUNC_(name,NAME) name ## _
  ```

  or

  ```
  #define SUNDIALS_CASE_LOWER 1
  #define SUNDIALS_UNDERSCORE_ONE 1
  ```

  in the sundials_config.h header file.

- Use of an MPI communicator other than MPI_COMM_WORLD in FORTRAN

  If the macro SUNDIALS_MPI_COMM_F2C is defined, then the MPI implementation used to build SUNDIALS defines the type MPI_Fint and the function MPI_Comm_f2c, and it is possible to use MPI communicators other than MPI_COMM_WORLD with the FORTRAN-C interface modules.

```
/*
 * -----------------------------------------------------------------
 * Copyright (c) 2005, The Regents of the University of California.
 * Produced at the Lawrence Livermore National Laboratory.
 * All rights reserved.
 * For details, see sundials/shared/LICENSE.
 * -----------------------------------------------------------------
 * SUNDIALS configuration header file
 * -----------------------------------------------------------------
 */


/* Define SUNDIALS version number
 * ------------------------------ */

#define SUNDIALS_PACKAGE_VERSION "2.2.1"

/* Define precision of SUNDIALS data type 'realtype'
 * ------------------------------------------------- */

/* Define SUNDIALS data type 'realtype' as 'double' */
#define SUNDIALS_DOUBLE_PRECISION 1

/* Define SUNDIALS data type 'realtype' as 'float' */
/* #define SUNDIALS_SINGLE_PRECISION 1 */

/* Define SUNDIALS data type 'realtype' as 'long double' */
/* #define SUNDIALS_EXTENDED_PRECISION 1 */

/* Use generic math functions
 * -------------------------- */

#define SUNDIALS_USE_GENERIC_MATH 1

/* FCMIX: Define Fortran name-mangling macro
 * ----------------------------------------- */

#define F77_FUNC(name,NAME) name ## _
#define F77_FUNC_(name,NAME) name ## _

/* FCMIX: Define case of function names
 * ----------------------------------- */

/* FCMIX: Make function names lowercase */
/* #define SUNDIALS_CASE_LOWER 1 */

/* FCMIX: Make function names uppercase */
/* #define SUNDIALS_CASE_UPPER 1 */

/* FCMIX: Define number of underscores to append to function names
 * -------------------------------------------------------------- */

/* FCMIX: Do NOT append any underscores to functions names */
/* #define SUNDIALS_UNDERSCORE_NONE 1 */

/* FCMIX: Append ONE underscore to function names */
/* #define SUNDIALS_UNDERSCORE_ONE 1 */

/* FCMIX: Append TWO underscores to function names */
/* #define SUNDIALS_UNDERSCORE_TWO 1 */

/* FNVECTOR: Allow user to specify different MPI communicator
 * ---------------------------------------------------------- */

#define SUNDIALS_MPI_COMM_F2C 1
```

Chapter 3

Mathematical Considerations

IDA solves the initial-value problem (IVP) for a DAE system of the general form

$$F(t, y, y') = 0\,, \quad y(t_0) = y_0\,,\ y'(t_0) = y'_0\,, \tag{3.1}$$

where y, y', and F are vectors in $\mathbf{R}^N$, t is the independent variable, $y' = dy/dt$, and initial values y_0, y'_0 are given. (Often t is time, but it certainly need not be.)

3.1 IVP solution

Prior to integrating a DAE initial-value problem, an important requirement is that the pair of vectors y_0 and y'_0 are both initialized to satisfy the DAE residual $F(t_0, y_0, y'_0) = 0$. For a class of problems that includes so-called semi-explicit index-one systems, IDA provides a routine that computes consistent initial conditions from a user's initial guess [4]. For this, the user must identify sub-vectors of y (not necessarily contiguous), denoted y_d and y_a, which are its differential and algebraic parts, respectively, such that F depends on y'_d but not on any components of y'_a. The assumption that the system is "index one" means that for a given t and y_d, the system $F(t, y, y') = 0$ defines y_a uniquely. In this case, a solver within IDA computes y_a and y'_d at $t = t_0$, given y_d and an initial guess for y_a. A second available option with this solver also computes all of $y(t_0)$ given $y'(t_0)$; this is intended mainly for quasi-steady-state problems, where $y'(t_0) = 0$ is given. In both cases, IDA solves the system $F(t_0, y_0, y'_0) = 0$ for the unknown components of y_0 and y'_0, using Newton iteration augmented with a line search global strategy. In doing this, it makes use of the existing machinery that is to be used for solving the linear systems during the integration, in combination with certain tricks involving the step size (which is set artificially for this calculation). For problems that do not fall into either of these categories, the user is responsible for passing consistent values or risk failure in the numerical integration.

The integration method used in IDA is the variable-order, variable-coefficient BDF (Backward Differentiation Formula), in fixed-leading-coefficient form [1]. The method order ranges from 1 to 5, with the BDF of order q given by the multistep formula

$$\sum_{i=0}^{q} \alpha_{n,i} y_{n-i} = h_n y'_n\,, \tag{3.2}$$

where y_n and y'_n are the computed approximations to $y(t_n)$ and $y'(t_n)$, respectively, and the step size is $h_n = t_n - t_{n-1}$. The coefficients $\alpha_{n,i}$ are uniquely determined by the order q, and the history of the step sizes. The application of the BDF (3.2) to the DAE system (3.1) results in a nonlinear algebraic system to be solved at each step:

$$G(y_n) \equiv F\left(t_n,\, y_n,\, h_n^{-1} \sum_{i=0}^{q} \alpha_{n,i} y_{n-i}\right) = 0\,. \tag{3.3}$$

Regardless of the method options, the solution of the nonlinear system (3.3) is accomplished with some form of Newton iteration. This leads to a linear system for each Newton correction, of the form

$$J[y_{n(m+1)} - y_{n(m)}] = -G(y_{n(m)}) \,, \tag{3.4}$$

where $y_{n(m)}$ is the m-th approximation to y_n. Here J is some approximation to the system Jacobian

$$J = \frac{\partial G}{\partial y} = \frac{\partial F}{\partial y} + \alpha \frac{\partial F}{\partial y'} \,, \tag{3.5}$$

where $\alpha = \alpha_{n,0}/h_n$. The scalar α changes whenever the step size or method order changes. The linear systems are solved by one of five methods:

- dense direct solver (serial version only),
- band direct solver (serial version only),
- diagonal approximate Jacobian solver,
- SPGMR = scaled preconditioned GMRES (Generalized Minimal Residual method) with restarts allowed,
- SPBCG = scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method), or
- SPTFQMR = scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method).

For the SPGMR, SPBCG, and SPTFQMR cases, preconditioning is allowed only on the left (see §3.2). Note that the direct linear solvers (dense and band) can only be used with serial vector representations.

In the process of controlling errors at various levels, IDA uses a weighted root-mean-square norm, denoted $\| \cdot \|_{\text{WRMS}}$, for all error-like quantities. The multiplicative weights used are based on the current solution and on the relative and absolute tolerances input by the user, namely

$$W_i = 1/[\text{RTOL} \cdot |y_i| + \text{ATOL}_i] \,. \tag{3.6}$$

Because $1/W_i$ represents a tolerance in the component y_i, a vector whose norm is 1 is regarded as "small." For brevity, we will usually drop the subscript WRMS on norms in what follows.

In the case of a direct linear solver (dense or banded), the nonlinear iteration (3.4) is a Modified Newton iteration, in that the Jacobian J is fixed (and usually out of date), with a coefficient $\bar{\alpha}$ in place of α in J. When using one of the Krylov methods SPGMR, SPBCG, or SPTFQMR as the linear solver, the iteration is an Inexact Newton iteration, using the current Jacobian (through matrix-free products Jv), in which the linear residual $J\Delta y + G$ is nonzero but controlled. The Jacobian matrix J (direct cases) or preconditioner matrix P (SPGMR/SPBCG/SPTFQMR case) is updated when:

- starting the problem,
- the value $\bar{\alpha}$ at the last update is such that $\alpha/\bar{\alpha} < 3/5$ or $\alpha/\bar{\alpha} > 5/3$, or
- a non-fatal convergence failure occurred with an out-of-date J or P.

The above strategy balances the high cost of frequent matrix evaluations and preprocessing with the slow convergence due to infrequent updates. To reduce storage costs on an update, Jacobian information is always reevaluated from scratch.

The stopping test for the Newton iteration in IDA ensures that the iteration error $y_n - y_{n(m)}$ is small relative to y itself. For this, we estimate the linear convergence rate at all iterations $m > 1$ as

$$R = \left(\frac{\delta_m}{\delta_1} \right)^{\frac{1}{m-1}} \,,$$

where the $\delta_m = y_{n(m)} - y_{n(m-1)}$ is the correction at iteration $m = 1, 2, \ldots$. The Newton iteration is halted if $R > 0.9$. The convergence test at the m-th iteration is then

$$S\|\delta_m\| < 0.33 \,, \tag{3.7}$$

where $S = R/(R-1)$ whenever $m > 1$ and $R \le 0.9$. The user has the option of changing the constant in the convergence test from its default value of 0.33. The quantity S is set to $S = 20$ initially and whenever J or P is updated, and it is reset to $S = 100$ on a step with $\alpha \ne \bar{\alpha}$. Note that at $m = 1$, the convergence test (3.7) uses an old value for S. Therefore, at the first Newton iteration, we make an additional test and stop the iteration if $\|\delta_1\| < 0.33 \cdot 10^{-4}$ (since such a δ_1 is probably just noise and therefore not appropriate for use in evaluating R). We allow only a small number (default value 4) of Newton iterations. If convergence fails with J or P current, we are forced to reduce the step size h_n, and we replace h_n by $h_n/4$. The integration is halted after a preset number (default value 10) of convergence failures. Both the maximum allowable Newton iterations and the maximum nonlinear convergence failures can be changed by the user from their default values.

When SPGMR, SPBCG, or SPTFQMR is used to solve the linear system, to minimize the effect of linear iteration errors on the nonlinear and local integration error controls, we require the preconditioned linear residual to be small relative to the allowed error in the Newton iteration, i.e., $\|P^{-1}(Jx+G)\| < 0.05 \cdot 0.33$. The safety factor 0.05 can be changed by the user.

In the direct linear solver cases, the Jacobian J defined in (3.5) can be either supplied by the user or have IDA compute one internally by difference quotients. In the latter case, we use the approximation

$$J_{ij} = [F_i(t, y + \sigma_j e_j, y' + \alpha\sigma_j e_j) - F_i(t, y, y')]/\sigma_j \,, \text{ with}$$
$$\sigma_j = \sqrt{U} \max\left\{|y_j|, |hy'_j|, 1/W_j\right\} \operatorname{sign}(hy'_j) \,,$$

where U is the unit roundoff, h is the current step size, and W_j is the error weight for the component y_j defined by (3.6). In the SPGMR/SPBCG/SPTFQMR case, if a routine for Jv is not supplied, such products are approximated by

$$Jv = [F(t, y + \sigma v, y' + \alpha\sigma v) - F(t, y, y')]/\sigma \,,$$

where the increment σ is $1/\|v\|$. As an option, the user can specify a constant factor that is inserted into this expression for σ.

During the course of integrating the system, IDA computes an estimate of the local truncation error, LTE, at the n-th time step, and requires this to satisfy the inequality

$$\|\text{LTE}\|_{\text{WRMS}} \le 1 \,.$$

Asymptotically, LTE varies as h^{q+1} at step size h and order q, as does the predictor-corrector difference $\Delta_n \equiv y_n - y_{n(0)}$. Thus there is a constant C such that

$$\text{LTE} = C\Delta_n + O(h^{q+2}) \,,$$

and so the norm of LTE is estimated as $|C| \cdot \|\Delta_n\|$. In addition, IDA requires that the error in the associated polynomial interpolant over the current step be bounded by 1 in norm. The leading term of the norm of this error is bounded by $\bar{C}\|\Delta_n\|$ for another constant $\bar{C}$. Thus the local error test in IDA is

$$\max\{|C|, \bar{C}\}\|\Delta_n\| \le 1 \,. \tag{3.8}$$

A user option is available by which the algebraic components of the error vector are omitted from the test (3.8), if these have been so identified.

In IDA, the local error test is tightly coupled with the logic for selecting the step size and order. First, there is an initial phase that is treated specially; for the first few steps, the step size is doubled and the order raised (from its initial value of 1) on every step, until (a) the local error test (3.8) fails, (b) the order is reduced (by the rules given below), or (c) the order reaches 5 (the maximum). For step and order selection on the general step, IDA uses a different set of local error estimates, based on the asymptotic behavior of the local error in the case of fixed step sizes. At each of the orders q' equal to q, $q-1$ (if $q > 1$), $q-2$ (if $q > 2$), or $q+1$ (if $q < 5$), there are constants $C(q')$ such that the norm of the local truncation error at order q' satisfies

$$\text{LTE}(q') = C(q')\|\phi(q'+1)\| + O(h^{q'+2}) \,,$$

where $\phi(k)$ is a modified divided difference of order k that is retained by IDA (and behaves asymptotically as h^k). Thus the local truncation errors are estimated as $\text{ELTE}(q') = C(q')\|\phi(q'+1)\|$ to select step sizes. But the choice of order in IDA is based on the requirement that the scaled derivative norms, $\|h^k y^{(k)}\|$, are monotonically decreasing with k, for k near q. These norms are again estimated using the $\phi(k)$, and in fact

$$\|h^{q'+1} y^{(q'+1)}\| \approx T(q') \equiv (q'+1)\text{ELTE}(q') \,.$$

The step/order selection begins with a test for monotonicity that is made even *before* the local error test is performed. Namely, the order is reset to $q' = q-1$ if (a) $q = 2$ and $T(1) \le T(2)/2$, or (b) $q > 2$ and $\max\{T(q-1), T(q-2)\} \le T(q)$; otherwise $q' = q$. Next the local error test (3.8) is performed, and if it fails, the step is redone at order $q \leftarrow q'$ and a new step size h'. The latter is based on the h^{q+1} asymptotic behavior of $\text{ELTE}(q)$, and, with safety factors, is given by

$$\eta = h'/h = 0.9/[2\,\text{ELTE}(q)]^{1/(q+1)} \,.$$

The value of η is adjusted so that $0.25 \le \eta \le 0.9$ before setting $h \leftarrow h' = \eta h$. If the local error test fails a second time, IDA uses $\eta = 0.25$, and on the third and subsequent failures it uses $q = 1$ and $\eta = 0.25$. After 10 failures, IDA returns with a give-up message.

As soon as the local error test has passed, the step and order for the next step may be adjusted. No such change is made if $q' = q-1$ from the prior test, if $q = 5$, or if q was increased on the previous step. Otherwise, if the last $q+1$ steps were taken at a constant order $q < 5$ and a constant step size, IDA considers raising the order to $q+1$. The logic is as follows: (a) If $q = 1$, then reset $q = 2$ if $T(2) < T(1)/2$. (b) If $q > 1$ then

- reset $q \leftarrow q-1$ if $T(q-1) \le \min\{T(q), T(q+1)\}$;
- else reset $q \leftarrow q+1$ if $T(q+1) < T(q)$;
- leave q unchanged otherwise [then $T(q-1) > T(q) \le T(q+1)$].

In any case, the new step size h' is set much as before:

$$\eta = h'/h = 1/[2\,\text{ELTE}(q)]^{1/(q+1)} \,.$$

The value of η is adjusted such that (a) if $\eta > 2$, η is reset to 2; (b) if $\eta \le 1$, η is restricted to $0.5 \le \eta \le 0.9$; and (c) if $1 < \eta < 2$ we use $\eta = 1$. Finally h is reset to $h' = \eta h$. Thus we do not increase the step size unless it can be doubled. See [1] for details.

IDA permits the user to impose optional inequality constraints on individual components of the solution vector y. Any of the following four constraints can be imposed: $y_i > 0$, $y_i < 0$, $y_i \ge 0$, or $y_i \le 0$. The constraint satisfaction is tested after a successful nonlinear system solution. If any constraint fails, we declare a convergence failure of the Newton iteration and reduce the step size. Rather than cutting the step size by some arbitrary factor, IDA estimates a new step size h' using a linear approximation of the components in y that failed the constraint test (including a safety factor of 0.9 to cover the strict inequality case). These additional constraints are also imposed during the calculation of consistent initial conditions.

Normally, IDA takes steps until a user-defined output value $t = t_{\text{out}}$ is overtaken, and then computes $y(t_{\text{out}})$ by interpolation. However, a "one step" mode option is available, where control returns to the calling program after each step. There are also options to force IDA not to integrate past a given stopping point $t = t_{\text{stop}}$.

3.2 Preconditioning

When using a Newton method to solve the nonlinear system (3.4), IDA makes repeated use of a linear solver to solve linear systems of the form $J\Delta y = -G$. If this linear system solve is done with one of the scaled preconditioned iterative linear solvers, these solvers are rarely successful if used without

preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system $Ax = b$ can be preconditioned on the left, on the right, or on both sides. The Krylov method is then applied to a system with the matrix $P^{-1}A$, or AP^{-1}, or $P_L^{-1}AP_R^{-1}$, instead of A. However, within IDA, preconditioning is allowed *only* on the left, so that the iterative method is applied to systems $(P^{-1}J)\Delta y = -P^{-1}G$. Left preconditioning is required to make the norm of the linear residual in the Newton iteration meaningful; in general, $\|J\Delta y + G\|$ is meaningless, since the weights used in the WRMS-norm correspond to y.

In order to improve the convergence of the Krylov iteration, the preconditioner matrix P should in some sense approximate the system matrix A. Yet at the same time, in order to be cost-effective, the matrix P should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [2] for an extensive study of preconditioners for reaction-transport systems).

Typical preconditioners used with IDA are based on approximations to the Newton iteration matrix of the systems involved; in other words, $P \approx \frac{\partial F}{\partial y} + \alpha\frac{\partial F}{\partial y'}$, where α is a scalar inverse proportional to the integration step size h. Because the Krylov iteration occurs within a Newton iteration and further also within a time integration, and since each of these iterations has its own test for convergence, the preconditioner may use a very crude approximation, as long as it captures the dominant numerical feature(s) of the system. We have found that the combination of a preconditioner with the Newton-Krylov iteration, using even a fairly poor approximation to the Jacobian, can be surprisingly superior to using the same matrix without Krylov acceleration (i.e., a modified Newton iteration), as well as to using the Newton-Krylov method with no preconditioning.

3.3 Rootfinding

The IDA solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (3.1), IDA can also find the roots of a set of user-defined functions $g_i(t, y, y')$ that depend on t, the solution vector $y = y(t)$, and its $t-$derivative $y'(t)$. The number of these root functions is arbitrary, and if more than one g_i is found to have a root in any given interval, the various root locations are found and reported in the order that they occur on the t axis, in the direction of integration.

Generally, this rootfinding feature finds only roots of odd multiplicity, corresponding to changes in sign of $g_i(t, y(t), y'(t))$, denoted $g_i(t)$ for short. If a user root function has a root of even multiplicity (no sign change), it will probably be missed by IDA. If such a root is desired, the user should reformulate the root function so that it changes sign at the desired root.

The basic scheme used is to check for sign changes of any $g_i(t)$ over each time step taken, and then (when a sign change is found) to home in on the root (or roots) with a modified secant method [11]. In addition, each time g is computed, IDA checks to see if $g_i(t) = 0$ exactly, and if so it reports this as a root. However, if an exact zero of any g_i is found at a point t, IDA computes g at $t + \delta$ for a small increment δ, slightly further in the direction of integration, and if any $g_i(t + \delta) = 0$ also, IDA stops and reports an error. This way, each time IDA takes a time step, it is guaranteed that the values of all g_i are nonzero at some past value of t, beyond which a search for roots is to be done.

At any given time in the course of the time-stepping, after suitable checking and adjusting has been done, IDA has an interval $(t_{lo}, t_{hi}]$ in which roots of the $g_i(t)$ are to be sought, such that t_{hi} is further ahead in the direction of integration, and all $g_i(t_{lo}) \neq 0$. The endpoint t_{hi} is either t_n, the end of the time step last taken, or the next requested output time $t_{\rm out}$ if this comes sooner. The endpoint t_{lo} is either t_{n-1}, or the last output time $t_{\rm out}$ (if this occurred within the last step), or the last root location (if a root was just located within this step), possibly adjusted slightly toward t_n if an exact zero was found. The algorithm checks g at t_{hi} for zeros and for sign changes in (t_{lo}, t_{hi}). If no sign changes are found, then either a root is reported (if some $g_i(t_{hi}) = 0$) or we proceed to the next time interval (starting at t_{hi}). If one or more sign changes were found, then a loop is entered to locate the root to within a rather tight tolerance, given by

$$\tau = 100 * U * (|t_n| + |h|) \quad (U = \text{unit roundoff}) \ .$$

Whenever sign changes are seen in two or more root functions, the one deemed most likely to have its root occur first is the one with the largest value of $|g_i(t_{hi})|/|g_i(t_{hi}) - g_i(t_{lo})|$, corresponding to the closest to t_{lo} of the secant method values. At each pass through the loop, a new value t_{mid} is set, strictly within the search interval, and the values of $g_i(t_{mid})$ are checked. Then either t_{lo} or t_{hi} is reset to t_{mid} according to which subinterval is found to have the sign change. If there is none in (t_{lo}, t_{mid}) but some $g_i(t_{mid}) = 0$, then that root is reported. The loop continues until $|t_{hi} - t_{lo}| < \tau$, and then the reported root location is t_{hi}.

In the loop to locate the root of $g_i(t)$, the formula for t_{mid} is

$$t_{mid} = t_{hi} - (t_{hi} - t_{lo})g_i(t_{hi})/[g_i(t_{hi}) - \alpha g_i(t_{lo})] \ ,$$

where α a weight parameter. On the first two passes through the loop, α is set to 1, making t_{mid} the secant method value. Thereafter, α is reset according to the side of the subinterval (low vs high, i.e. toward t_{lo} vs toward t_{hi}) in which the sign change was found in the previous two passes. If the two sides were opposite, α is set to 1. If the two sides were the same, α is halved (if on the low side) or doubled (if on the high side). The value of t_{mid} is closer to t_{lo} when $\alpha < 1$ and closer to t_{hi} when $\alpha > 1$. If the above value of t_{mid} is within $\tau/2$ of t_{lo} or t_{hi}, it is adjusted inward, such that its fractional distance from the endpoint (relative to the interval size) is between .1 and .5 (.5 being the midpoint), and the actual distance from the endpoint is at least $\tau/2$.

Chapter 4

Code Organization

4.1 SUNDIALS organization

The family of solvers referred to as SUNDIALS consists of the solvers CVODE (for ODE systems), KINSOL (for nonlinear algebraic systems), and IDA (for differential-algebraic systems). In addition, variants of these which also do sensitivity analysis calculations are available or in development. CVODES, an extension of CVODE that provides both forward and adjoint sensitivity capabilities is available, while IDAS is currently in development.

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Fig. 4.1). The following is a list of the solver packages presently available:

- CVODE, a solver for stiff and nonstiff ODEs $dy/dt = f(t, y)$;
- CVODES, a solver for stiff and nonstiff ODEs $dy/dt = f(t, y, p)$ with sensitivity analysis capabilities;
- KINSOL, a solver for nonlinear algebraic systems $F(u) = 0$;
- IDA, a solver for differential-algebraic systems $F(t, y, y') = 0$.

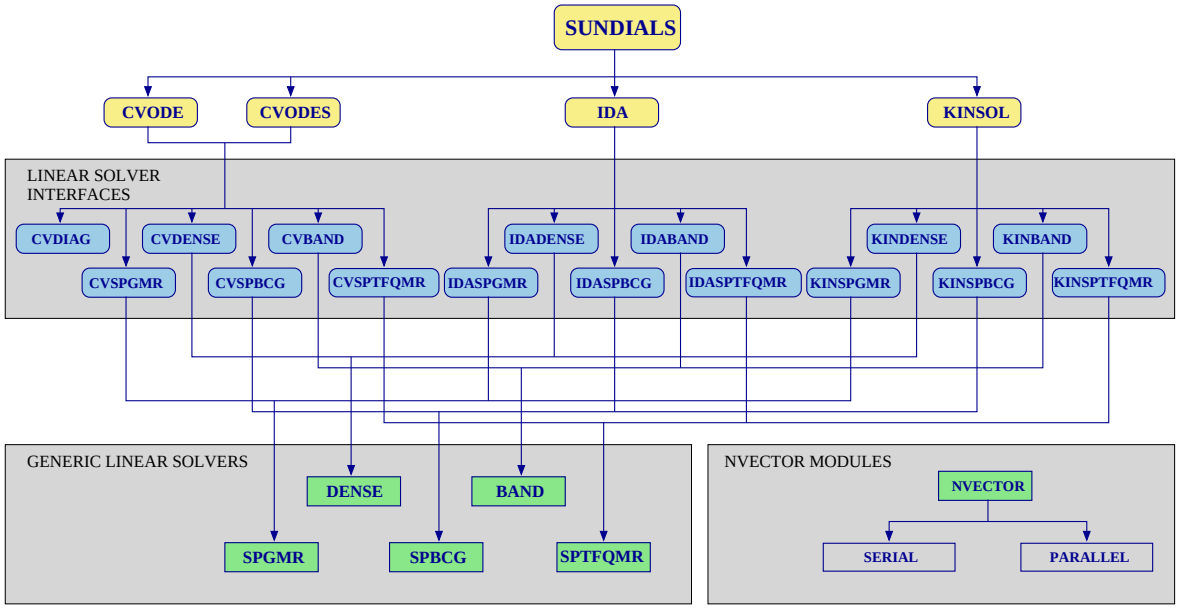
4.2 IDA organization

The IDA package is written in the ANSI C language. The following summarizes the basic structure of the package, although knowledge of this structure is not necessary for its use.

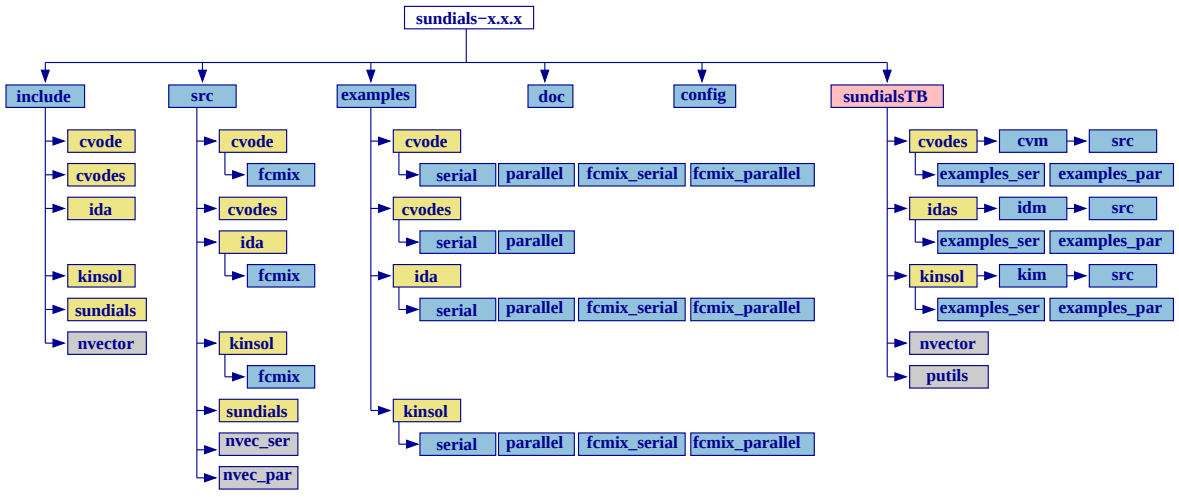
The overall organization of the IDA package is shown in Figure 4.2. The central integration module, implemented in the files `ida.h`, `ida_impl.h`, and `ida.c`, deals with the evaluation of integration coefficients, the Newton iteration process, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues. Although this module contains logic for the basic Newton iteration algorithm, it has no knowledge of the method being used to solve the linear systems that arise. For any given user problem, one of the linear system modules is specified, and is then invoked as needed during the integration.

At present, the package includes the following five IDA linear system modules:

- IDADENSE: LU factorization and backsolving with dense matrices;
- IDABAND: LU factorization and backsolving with banded matrices;
- IDASPGMR: scaled preconditioned GMRES method;
- IDASPBCG: scaled preconditioned Bi-CGStab method;
- IDASPTFQMR: scaled preconditioned TFQMR method.



(a) High-level diagram



(b) Directory structure of the source tree

Figure 4.1: Organization of the SUNDIALS suite

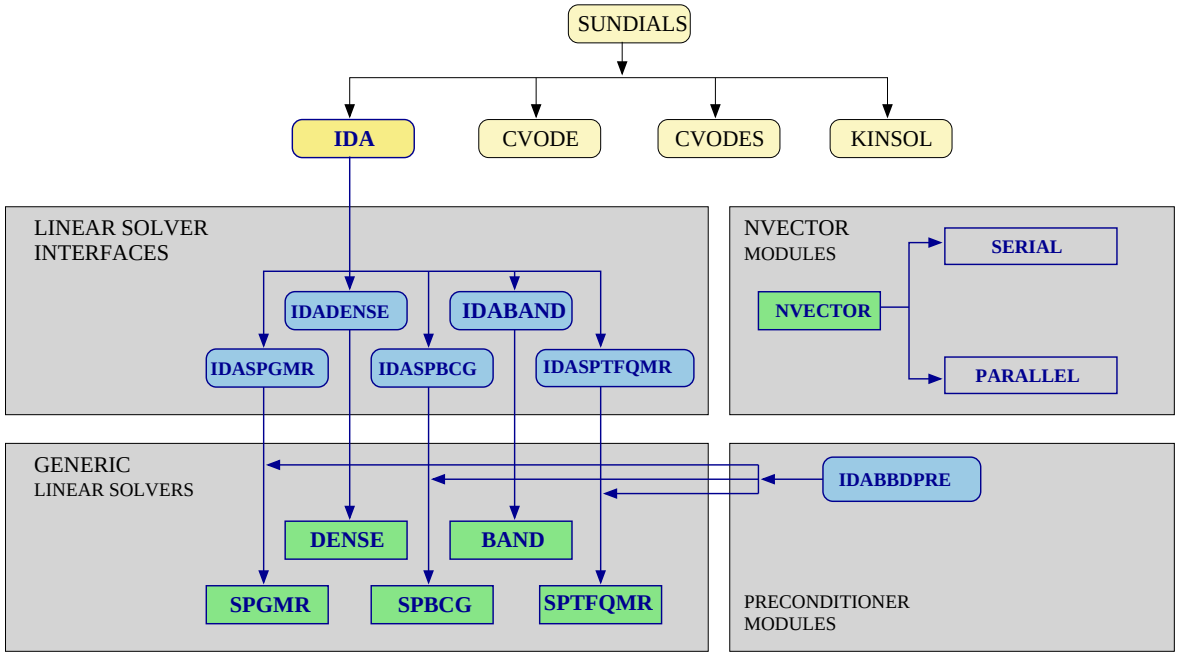


Figure 4.2: Overall structure diagram of the IDA package. Modules specific to IDA are distinguished by rounded boxes, while generic solver and auxiliary modules are in square boxes.

This set of linear solver modules is intended to be expanded in the future as new algorithms are developed.

In the case of the direct methods IDADENSE and IDABAND, the package includes an algorithm for the approximation of the Jacobian by difference quotients, but the user also has the option of supplying the Jacobian (or an approximation to it) directly. In the case of the Krylov iterative methods IDASPGMR, IDASPBCG, and IDASPTFQMR, the package includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector of appropriate length. Again, the user has the option of providing a routine for this operation. When using any of the Krylov methods, the user must supply the preconditioning in two phases: a setup phase (preprocessing of Jacobian data) and a solve phase. While there is no default choice of preconditioner analogous to the difference quotient approximation in the direct case, the references [2, 5], together with the example and demonstration programs included with IDA, offer considerable assistance in building preconditioners.

Each IDA linear solver module consists of five routines, devoted to (1) memory allocation and initialization, (2) setup of the matrix data involved, (3) solution of the system, (4) monitoring performance, and (5) freeing of memory. The setup and solution phases are separate because the evaluation of Jacobians and preconditioners is done only periodically during the integration, as required to achieve convergence. The call list within the central IDA module to each of the five associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

These modules are also decomposed in another way. Each of the modules IDADENSE, IDABAND, IDASPGMR, IDASPBCG, and IDASPTFQMR is a set of interface routines built on top of a generic solver module, named DENSE, BAND, SPGMR, SPBCG, and SPTFQMR, respectively. The interfaces deal with the use of these methods in the IDA context, whereas the generic solver is independent of the context. While the generic solvers here were generated with SUNDIALS in mind, our intention is that they be usable in other applications as general-purpose solvers. This separation also allows for any generic solver to be replaced by an improved version, with no necessity to revise the IDA package elsewhere.

IDA also provides a preconditioner module, IDABBDPRE, that works in conjunction with NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix.

All state information used by IDA to solve a given problem is saved in a structure, and a pointer to that structure is returned to the user. There is no global data in the IDA package, and so in this respect it is reentrant. State information specific to the linear solver is saved in a separate structure, a pointer to which resides in the IDA memory structure. The reentrancy of IDA was motivated by the situation where two or more problems are solved by intermixed calls to the package from one user program.

Chapter 5

Using IDA for C Applications

This chapter is concerned with the use of IDA for the integration of DAEs. The following sections treat the header files, the layout of the user's main program, description of the IDA user-callable functions, and description of user-supplied functions. The listings of the sample programs in the companion document [13] may also be helpful. Those codes may be used as templates (with the removal of some lines involved in testing), and are included in the IDA package.

The user should be aware that not all linear solver modules are compatible with all NVECTOR implementations. For example, NVECTOR_PARALLEL is not compatible with the direct dense or direct band linear solvers, since these linear solver modules need to form the complete system Jacobian. The IDADENSE and IDABAND modules can only be used with NVECTOR_SERIAL. The preconditioner module IDABBDPRE can only be used with NVECTOR_PARALLEL.

IDA uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in Chapter 10.

5.1 Access to library and header files

At this point, it is assumed that the installation of IDA, following the procedure described in Chapter 2, has been completed successfully.

Regardless of where the user's application program resides, its associated compilation and load commands must make reference to the appropriate locations for the library and header files required by IDA. The relevant library files are

- *libdir*`/libsundials_ida.`*lib*,
- *libdir*`/libsundials_nvec*.`*lib* (one or two files),

where the file extension *.lib* is typically `.so` for shared libraries and `.a` for static libraries. The relevant header files are located in the subdirectories

- *incdir*`/include`
- *incdir*`/include/ida`
- *incdir*`/include/sundials`

The directories *libdir* and *incdir* are the install libray and include directories. For a default installation, these are *builddir*`/lib` and *builddir*`/include`, respectively, where *builddir* was defined in Chapter 2.

5.2 Data types

The `sundials_types.h` file contains the definition of the type `realtype`, which is used by the SUNDIALS solvers for all floating-point data. The type `realtype` can be `float`, `double`, or `long double`, with

the default being `double`. The user can change the precision of the SUNDIALS solvers arithmetic at the configuration stage (see §2.1).

Additionally, based on the current precision, `sundials_types.h` defines `BIG_REAL` to be the largest value representable as a `realtype`, `SMALL_REAL` to be the smallest value representable as a `realtype`, and `UNIT_ROUNDOFF` to be the difference between 1.0 and the minimum `realtype` greater than 1.0.

Within SUNDIALS, real constants are set by way of a macro called `RCONST`. It is this macro that needs the ability to branch on the definition `realtype`. In ANSI C, a floating-point constant with no suffix is stored as a `double`. Placing the suffix "F" at the end of a floating point constant makes it a `float`, whereas using the suffix "L" makes it a `long double`. For example,

```
#define A 1.0
#define B 1.0F
#define C 1.0L
```

defines `A` to be a `double` constant equal to 1.0, `B` to be a `float` constant equal to 1.0, and `C` to be a `long double` constant equal to 1.0. The macro call `RCONST(1.0)` automatically expands to `1.0` if `realtype` is `double`, to `1.0F` if `realtype` is `float`, or to `1.0L` if `realtype` is `long double`. SUNDIALS uses the `RCONST` macro internally to declare all of its floating-point constants.

A user program which uses the type `realtype` and the `RCONST` macro to handle floating-point constants is precision-independent except for any calls to precision-specific standard math library functions. (Our example programs use both `realtype` and `RCONST`.) Users can, however, use the type `double`, `float`, or `long double` in their code (assuming the typedef for `realtype` matches this choice). Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use `realtype`, so long as the SUNDIALS libraries use the correct precision (for details see §2.1).

5.3 Header files

The calling program must include several header files so that various macros and data types can be used. The header file that is always required is:

- `ida.h`, the header file for IDA, which defines the several types and various constants, and includes function prototypes.

Note that `ida.h` includes `sundials_types.h`, which defines the types `realtype` and `booleantype` and the constants `FALSE` and `TRUE`.

The calling program must also include an NVECTOR implementation header file (see Chapter 7 for details). For the two NVECTOR implementations that are included in the IDA package, the corresponding header files are:

- `nvector_serial.h`, which defines the serial implementation NVECTOR_SERIAL;
- `nvector_parallel.h`, which defines the parallel MPI implementation, NVECTOR_PARALLEL.

Note that both these files include in turn the header file `sundials_nvector.h` which defines the abstract `N_Vector` type.

Finally, a linear solver module header file is required. The header files corresponding to the various linear solver options in IDA are as follows:

- `ida_dense.h`, which is used with the dense direct linear solver in the context of IDA. This in turn includes a header file (`sundials_dense.h`) which defines the `DenseMat` type and corresponding accessor macros;
- `ida_band.h`, which is used with the band direct linear solver in the context of IDA. This in turn includes a header file (`sundials_band.h`) which defines the `BandMat` type and corresponding accessor macros;
- `ida_spgmr.h`, which is used with the Krylov solver SPGMR in the context of IDA;

- `ida_spbcgs.h`, which is used with the Krylov solver SPBCG in the context of IDA;
- `ida_sptfqmr.h`, which is used with the Krylov solver SPTFQMR in the context of IDA;

The header files for the Krylov iterative solvers include `ida_spils.h` which defined common fu-unctions and which in turn includes a header file (`sundials_iterative.h`) which enumerates the kind of preconditioning and for the choices for the Gram-Schmidt process for SPGMR.

5.4 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the integration of a DAE IVP. Some steps are independent of the NVECTOR implementation used; where this is not the case, usage specifications are given for the two implementations provided with IDA: steps marked with [**P**] correspond to NVECTOR_PARALLEL, while steps marked with [**S**] correspond to NVECTOR_SERIAL.

1. **[P] Initialize MPI**

   Call `MPI_Init(&argc, &argv);` to initialize MPI if used by the user's program, aside from the internal use in NVECTOR_PARALLEL. Here `argc` and `argv` are the command line argument counter and array received by `main`.

2. **Set problem dimensions**

   [**S**] Set `N`, the problem size N.

   [**P**] Set `Nlocal`, the local vector length (the sub-vector length for this processor); `N`, the global vector length (the problem size N, and the sum of all the values of `Nlocal`); and the active set of processors.

3. **Set vector of initial values**

   To set the vectors `y0` and `yp0` to initial values for y and y', use functions defined by a particular NVECTOR implementation. For the two NVECTOR implementations provided, if a `realtype` array `ydata` already exists, containing the initial values of y, make the call:

   [**S**] `y0 = N_VMake_Serial(N, ydata);`

   [**P**] `y0 = N_VMake_Parallel(comm, Nlocal, N, ydata);`

   Otherwise, make the call:

   [**S**] `y0 = N_VNew_Serial(N);`

   [**P**] `y0 = N_VNew_Parallel(comm, Nlocal, N);`

   and load initial values into the structure defined by:

   [**S**] `NV_DATA_S(y0)`

   [**P**] `NV_DATA_P(y0)`

   Here `comm` is the MPI communicator, set in one of two ways: If a proper subset of active processors is to be used, `comm` must be set by suitable MPI calls. Otherwise, to specify that all processors are to be used, `comm` must be `MPI_COMM_WORLD`.

   The initial conditions for y' are set similarly.

4. **Create IDA object**

   Call `ida_mem = IDACreate();` to create the IDA memory block. `IDACreate` returns a pointer to the IDA memory structure. See §5.5.1 for details.

5. **Allocate internal memory**

Call `IDAMalloc(...);` to provide required problem specifications, allocate internal memory for IDA, and initialize IDA. `IDAMalloc` returns an error flag to indicate success or an illegal argument value. See §5.5.1 for details.

6. **Set optional inputs**

   Call `IDASet*` functions to change from their default values any optional inputs that control the behavior of IDA. See §5.5.6.1 for details.

7. **Attach linear solver module**

   Initialize the linear solver module with one of the following calls (for details see §5.5.3):

   [**S**] `flag = IDADense(...);`

   [**S**] `flag = IDABand(...);`

   `flag = IDASpgmr(...);`

   `flag = IDASpbcg(...);`

   `flag = IDASptfqmr(...);`

8. **Set linear solver optional inputs**

   Call `IDA*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See §5.5.6.3 for details.

9. **Correct initial values**

   Optionally, call `IDACalcIC` to correct the initial values `y0` and `yp0` passed to `IDAMalloc`. See §5.5.4. Also see §5.5.6.2 for relevant optional input calls.

10. **Specify rootfinding problem**

    Optionally, call `IDARootInit` to initialize a rootfinding problem to be solved during the integration of the DAE system. See §5.7.1 for details.

11. **Advance solution in time**

    For each point at which output is desired, call `flag = IDASolve(ida_mem, tout, &tret, yret, ypret, itask);` Set `itask` to specify the return mode. The vector `yret` (which can be the same as the vector `y0` above) will contain $y(t)$, while the vector `ypret` will contain $y'(t)$. See §5.5.5 for details.

12. **Get optional outputs**

    Call `IDA*Get*` functions to obtain optional output. See §5.5.8 and §5.7.1 for details.

13. **Deallocate memory for solution vector**

    Upon completion of the integration, deallocate memory for the vectors `yret` and `ypret` by calling the destructor function defined by the NVECTOR implementation:

    [**S**] `N_VDestroy_Serial(yret);`

    [**P**] `N_VDestroy_Parallel(yret);`

    and similarly for `ypret`.

14. **Free solver memory**

    `IDAFree(&ida_mem);` to free the memory allocated for IDA.

15. **[P] Finalize MPI**

    Call `MPI_Finalize();` to terminate MPI.

5.5 User-callable functions

This section describes the IDA functions that are called by the user to set up and solve a DAE. Some of these are required. However, starting with §5.5.6, the functions listed involve optional inputs/outputs or restarting, and those paragraphs can be skipped for a casual use of IDA. In any case, refer to §5.4 for the correct order of these calls. Calls related to rootfinding are described in §5.7.

5.5.1 IDA initialization and deallocation functions

The following three functions must be called in the order listed. The last one is to be called only after the DAE solution is complete, as it frees the IDA memory block created and allocated by the first two calls.

`IDACreate`

Call `ida_mem = IDACreate();`

Description The function `IDACreate` instantiates an IDA solver object.

Arguments `IDACreate` has no arguments.

Return value If successful, `IDACreate` returns a pointer to the newly created IDA memory block (of type `void *`). If an error occurred, `IDACreate` prints an error message to `stderr` and returns `NULL`.

`IDAMalloc`

Call `flag = IDAMalloc(ida_mem, res, t0, y0, yp0, itol, reltol, abstol);`

Description The function `IDAMalloc` provides required problem and solution specifications, allocates internal memory, and initializes IDA.

Arguments

`ida_mem` (`void *`) pointer to the IDA memory block returned by `IDACreate`.

`res` (`IDAResFn`) is the C function which computes F in the DAE. This function has the form `res(t, yy, yp, resval, res_data)` (for full details see §5.6).

`t0` (`realtype`) is the initial value of t.

`y0` (`N_Vector`) is the initial value of y.

`yp0` (`N_Vector`) is the initial value of y'.

`itol` (`int`) is one of `IDA_SS`, `IDA_SV`, or `IDA_WF`. Here `itol` = `IDA_SS` indicates scalar relative error tolerance and scalar absolute error tolerance, while `itol` = `IDA_SV` indicates scalar relative error tolerance and vector absolute error tolerance. The latter choice is important when the absolute error tolerance needs to be different for each component of the DAE. If `itol` = `IDA_WF`, the arguments `reltol` and `abstol` are ignored and the user is expected to provide a function to evaluate the error weight vector W, replacing (3.6). See `IDASetEwtFn` in §5.5.6.1.

`reltol` (`realtype`) is the relative error tolerance.

`abstol` (`void *`) is a pointer to the absolute error tolerance. If `itol` = `IDA_SS`, `abstol` must be a pointer to a `realtype` variable. If `itol` = `IDA_SV`, `abstol` must be an `N_Vector` variable.

Return value The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS` The call to `IDAMalloc` was successful.

`IDA_MEM_NULL` The IDA memory block was not initialized through a previous call to `IDACreate`.

`IDA_MEM_FAIL` A memory allocation request has failed.

`IDA_ILL_INPUT` An input argument to `IDAMalloc` has an illegal value.

Notes See also §5.5.2 for advice on tolerances.

The tolerance values in `reltol` and `abstol` may be changed between calls to `IDASolve` (see `IDASetTolerances` in §5.5.6.1).

It is the user's responsibility to provide compatible `itol` and `abstol` arguments.

If an error occurred, `IDAMalloc` also sends an error message to the error handler function.

`IDAFree`

Call `IDAFree(&ida_mem);`

Description The function `IDAFree` frees the pointer allocated by a previous call to `IDAMalloc`.

Arguments The argument is the pointer to the IDA memory block (of type `void *`).

Return value The function `IDAFree` has no return value.

5.5.2 Advice on choice and use of tolerances

General advice on choice of tolerances. For many users, the appropriate choices for tolerance values in `reltol` and `abstol` are a concern. The following pieces of advice are relevant.

(1) The scalar relative tolerance `reltol` is to be set to control relative errors. So `reltol` = 1.0E-4 means that errors are controlled to .01%. We do not recommend using `reltol` larger than 1.0E-3. On the other hand, `reltol` should not be so small that it is comparable to the unit roundoff of the machine arithmetic (generally around 1.0E-15).

(2) The absolute tolerances `abstol` (whether scalar or vector) need to be set to control absolute errors when any components of the solution vector `y` may be so small that pure relative error control is meaningless. For example, if `y[i]` starts at some nonzero value, but in time decays to zero, then pure relative error control on `y[i]` makes no sense (and is overly costly) after `y[i]` is below some noise level. Then `abstol` (if scalar) or `abstol[i]` (if a vector) needs to be set to that noise level. If the different components have different noise levels, then `abstol` should be a vector. See the example `idadenx` in the IDA package, and the discussion of it in the IDA Examples document [13]. In that problem, the three components vary betwen 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

(3) Finally, it is important to pick all the tolerance values conservately, because they control the error committed on each individual time step. The final (global) errors are some sort of accumulation of those per-step errors. A good rule of thumb is to reduce the tolerances by a factor of .01 from the actual desired limits on errors. So if you want .01% accuracy (globally), a good choice is `reltol` = 1.0E-6. But in any case, it is a good idea to do a few experiments with the tolerances to see how the computed solution values vary as tolerances are reduced.

Advice on controlling unphysical negative values. In many applications, some components in the true solution are always positive or non-negative, though at times very small. In the numerical solution, however, small negative (hence unphysical) values can then occur. In most cases, these values are harmless, and simply need to be controlled, not eliminated. The following pieces of advice are relevant.

(1) The way to control the size of unwanted negative computed values is with tighter absolute tolerances. Again this requires some knowledge of the noise level of these components, which may or may not be different for different components. Some experimentation may be needed.

(2) If output plots or tables are being generated, and it is important to avoid having negative numbers appear there (for the sake of avoiding a long explanation of them, if nothing else), then eliminate them, but only in the context of the output medium. Then the internal values carried by the solver are unaffected. Remember that a small negative value in `yret` returned by IDA, with magnitude comparable to `abstol` or less, is equivalent to zero as far as the computation is concerned.

(3) The user's residual routine `res` should never change a negative value in the solution vector `yy` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `res` routine cannot tolerate a zero or negative value (e.g. because there is a square root or log of it), then the offending value should be changed to zero or a tiny positive number in a temporary variable (not in the input `yy` vector) for the purposes of computing $F(t, y)$.

(4) IDA provides the option of enforcing positivity or non-negativity on components. But these constraint options should only be exercised if the use of absolute tolerances to control the computed values is unsuccessful, because they involve some extra overhead cost.

5.5.3 Linear solver specification functions

As previously explained, Newton iteration requires the solution of linear systems of the form (3.4). There are five IDA linear solvers currently available for this task: IDADENSE, IDABAND, IDASPGMR, IDASPBCG, and IDASPTFQMR. The first two are direct solvers and derive their name from the type of approximation used for the Jacobian $J = \partial F/\partial y + c_j \partial F/\partial y'$. IDADENSE and IDABAND work with dense and banded approximations to J, respectively. The remaining three IDA linear solvers, IDASPGMR, IDASPBCG, and IDASPTFQMR, are Krylov iterative solvers. The SPGMR, SPBCG, and SPTFQMR in the names indicate the scaled preconditioned GMRES, scaled preconditioned Bi-CGStab, and scaled preconditioned TFQMR methods, respectively. Together, they are refered to as IDASPILS (from scaled preconditioned iterative linear solvers).

When using any of the Krylov linear solvers, preconditioning (on the left) is permitted, and in fact encouraged, for the sake of efficiency. A preconditioner matrix P must approximate the Jacobian J, at least crudely. For the specification of a preconditioner, see §5.5.6.3 and §5.6.

To specify an IDA linear solver, after the call to `IDACreate` but before any calls to `IDASolve`, the user's program must call one of the functions `IDADense`, `IDABand`, `IDASpgmr`, `IDASpbcg`, or `IDASptfqmr`, as documented below. The first argument passed to these functions is the IDA memory pointer returned by `IDACreate`. A call to one of these functions links the main IDA integrator to a linear solver and allows the user to specify parameters which are specific to a particular solver, such as the bandwidths in the IDABAND case. The use of each of the linear solvers involves certain constants and possibly some macros, that are likely to be needed in the user code. These are available in the corresponding header file associated with the linear solver, as specified below.

In each case the linear solver module used by IDA is actually built on top of a generic linear system solver, which may be of interest in itself. These generic solvers, denoted DENSE, BAND, SPGMR, SPBCG, and SPTFQMR, are described separately in Chapter 9.

`IDADense`

Call `flag = IDADense(ida_mem, N);`

Description The function `IDADense` selects the IDADENSE linear solver.

The user's main function must include the `ida_dense.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`N` (`long int`) problem dimension.

Return value The return value `flag` (of type `int`) is one of

`IDADENSE_SUCCESS`	The IDADENSE initialization was successful.
`IDADENSE_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADENSE_ILL_INPUT`	The IDADENSE solver is not compatible with the current NVECTOR module.
`IDADENSE_MEM_FAIL`	A memory allocation request failed.

Notes The IDADENSE linear solver may not be compatible with a particular implementation of the NVECTOR module. Of the two NVECTOR modules provided by SUNDIALS, only NVECTOR_SERIAL is compatible, while NVECTOR_PARALLEL is not.

`IDABand`

Call `flag = IDABand(ida_mem, N, mupper, mlower);`

Description The function `IDABand` selects the IDABAND linear solver.

The user's main function must include the `ida_band.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`N` (`long int`) problem dimension.

`mupper` (`long int`) upper half-bandwidth of the problem Jacobian (or of the approximation of it).

`mlower` (`long int`) lower half-bandwidth of the problem Jacobian (or of the approximation of it).

Return value The return value `flag` (of type `int`) is one of

`IDABAND_SUCCESS` The IDABAND initialization was successful.

`IDABAND_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDABAND_ILL_INPUT` The IDABAND solver is not compatible with the current NVECTOR module, or one of the Jacobian half-bandwidths is outside its valid range ($0 \ldots$ `N`-1).

`IDABAND_MEM_FAIL` A memory allocation request failed.

Notes The IDABAND linear solver may not be compatible with a particular implementation of the NVECTOR module. Of the two NVECTOR modules provided by SUNDIALS, only NVECTOR_SERIAL is compatible, while NVECTOR_PARALLEL is not. The half-bandwidths are to be set so that the nonzero locations (i, j) in the banded (approximate) Jacobian satisfy $-$`mlower` $\leq j - i \leq$ `mupper`.

`IDASpgmr`

Call `flag = IDASpgmr(ida_mem, maxl);`

Description The function `IDASpgmr` selects the IDASPGMR linear solver.

The user's main function must include the `ida_spgmr.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPGMR_MAXL`$= 5$.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPGMR initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

`IDASpbcg`

Call `flag = IDASpbcg(ida_mem, maxl);`

Description The function `IDASpbcg` selects the IDASPBCG linear solver.

The user's main function must include the `ida_spbcgs.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPBCG_MAXL`$= 5$.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPBCG initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

IDASptfqmr

Call `flag = IDASptfqmr(ida_mem, maxl);`

Description The function `IDASptfqmr` selects the IDASPTFQMR linear solver.

The user's main function must include the `ida_sptfqmr.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPTFQMR_MAXL`= 5.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPTFQMR initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

5.5.4 Initial condition calculation function

`IDACalcIC` calculates corrected initial conditions for the DAE system for a class of index-one problems of semi-implicit form. (See §3.1 and Ref. [4].) It uses Newton iteration combined with a linesearch algorithm. Calling `IDACalcIC` is optional. It is only necessary when the initial conditions do not solve the given system. Thus if `y0` and `yp0` are known to satisfy $F(t_0, y_0, y_0') = 0$, then a call to `IDACalcIC` is generally *not* necessary.

A call to `IDACalcIC` must be preceded by successful calls to `IDACreate` and `IDAMalloc` (or `IDAReInit`), and by a successful call to the linear system solver specification function. The call to `IDACalcIC` should precede the call(s) to `IDASolve` for the given problem.

IDACalcIC

Call `flag = IDACalcIC(ida_mem, icopt, tout1);`

Description The function `IDACalcIC` corrects the initial values `y0` and `yp0` at time `t0`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`icopt` (`int`) is one of the following two options for the initial condition calculation.

`icopt=IDA_YA_YDP_INIT` directs `IDACalcIC` to compute the algebraic components of y and differential components of y', given the differential components of y. This option requires that the `N_Vector id` was set through `IDASetId`, specifying the differential and algebraic components.

`icopt=IDA_Y_INIT` directs `IDACalcIC` to compute all components of y, given y'. In this case, `id` is not required.

`tout1` (`realtype`) is the first value of t at which a solution will be requested (from `IDASolve`). This value is needed here to determine the direction of integration and rough scale in the independent variable t.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	`IDASolve` succeeded.
`IDA_MEM_NULL`	The argument `ida_mem` was `NULL`.
`IDA_NO_MALLOC`	The allocation function `IDAMalloc` has not been called.
`IDA_ILL_INPUT`	One of the input arguments was illegal.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_LINIT_FAIL`	The linear solver's initialization function failed.
`IDA_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.

IDA_BAD_EWT	Some component of the error weight vector is zero (illegal), either for the input value of y0 or a corrected value.
IDA_FIRST_RES_FAIL	The user's residual function returned a recoverable error flag on the first call, but IDACalcIC was unable to recover.
IDA_RES_FAIL	The user's residual function returned a nonrecoverable error flag.
IDA_NO_RECOVERY	The user's residual function, or the linear solver's setup or solve function had a recoverable error, but IDACalcIC was unable to recover.
IDA_CONSTR_FAIL	IDACalcIC was unable to find a solution satisfying the inequality constraints.
IDA_LINESEARCH_FAIL	The linesearch algorithm failed to find a solution with a step larger than steptol in weighted RMS norm.
IDA_CONV_FAIL	IDACalcIC failed to get convergence of the Newton iterations.

Notes All failure return values are negative and therefore a test `flag` < 0 will trap all IDACalcIC failures.

Note that IDACalcIC will correct the values $y(t_0)$ and $y'(t_0)$ which were specified in the previous call to IDAMalloc or IDAReInit. To obtain the corrected values, call IDAGetconsistentIC (see §5.5.8.2).

5.5.5 IDA solver function

This is the central step in the solution process — the call to perform the integration of the DAE.

IDASolve

Call `flag = IDASolve(ida_mem, tout, tret, yret, ypret, itask);`

Description The function IDASolve integrates the DAE over an interval in t.

Arguments

ida_mem	(void *) pointer to the IDA memory block.
tout	(realtype) the next time at which a computed solution is desired.
tret	(realtype *) the time reached by the solver.
yret	(N_Vector) the computed solution vector y.
ypret	(N_Vector) the computed solution vector y'.
itask	(int) a flag indicating the job of the solver for the next user step. The IDA_NORMAL task is to have the solver take internal steps until it has reached or just passed the user specified tout parameter. The solver then interpolates in order to return approximate values of y(tout) and y'(tout). The IDA_ONE_STEP option tells the solver to just take one internal step and return the solution at the point reached by that step. The IDA_NORMAL_TSTOP and IDA_ONE_STEP_TSTOP modes are similar to IDA_NORMAL and IDA_ONE_STEP, respectively, except that the integration never proceeds past the value tstop, specified through the function IDASetStopTime (see §5.5.6.1).

Return value On return, IDASolve returns vectors yret and ypret and a corresponding independent variable value t =*tret, such that (yret, ypret) are the computed values of ($y(t)$, $y'(t)$).

In IDA_NORMAL mode with no errors, *tret will be equal to tout and yret = y(tout), ypret = y'(tout).

The return value flag (of type int) will be one of the following:

IDA_SUCCESS	IDASolve succeeded.
IDA_TSTOP_RETURN	IDASolve succeeded by reaching the stop point specified through the optional input function IDASetStopTime.

IDA_ROOT_RETURN	IDASolve succeeded and found one or more roots. If nrtfn > 1, call IDAGetRootInfo to see which g_i were found to have a root. See §5.7 for more information.
IDA_MEM_NULL	The ida_mem argument was NULL.
IDA_ILL_INPUT	One of the inputs to IDASolve is illegal. This includes the situation where a root of one of the root functions was found both at a point t and also very near t. It also includes the situation when a component of the error weight vectors becomes negative during internal time-stepping. The IDA_ILL_INPUT flag will also be returned if the linear solver function initialization (called by the user after calling IDACreate) failed to set the linear solver-specific lsolve field in ida_mem. In any case, the user should see the printed error message for more details.
IDA_TOO_MUCH_WORK	The solver took mxstep internal steps but could not reach tout. The default value for mxstep is MXSTEP_DEFAULT = 500.
IDA_TOO_MUCH_ACC	The solver could not satisfy the accuracy demanded by the user for some internal step.
IDA_ERR_FAIL	Error test failures occurred too many times (MXNEF = 10) during one internal time step or occurred with $\|h\| = h_{min}$.
IDA_CONV_FAIL	Convergence test failures occurred too many times (MXNCF = 10) during one internal time step or occurred with $\|h\| = h_{min}$.
IDA_LINIT_FAIL	The linear solver's initialization function failed.
IDA_LSETUP_FAIL	The linear solver's setup function failed in an unrecoverable manner.
IDA_LSOLVE_FAIL	The linear solver's solve function failed in an unrecoverable manner.
IDA_CONSTR_FAIL	The inequality constraints were violated and the solver was unable to recover.
IDA_REP_RES_ERR	The user's residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_RES_FAIL	The user's residual function returned a nonrecoverable error flag.
IDA_RTFUNC_FAIL	The rootfinding function failed.

Notes

The vector yret can occupy the same space as the y0 vector of initial conditions that was passed to IDAMalloc, while the vector ypret can occupy the same space as the yp0.

In the IDA_ONE_STEP mode, tout is used on the first call only, to get the direction and rough scale of the independent variable.

All failure return values are negative and therefore a test flag < 0 will trap all IDASolve failures.

On any error return in which one or more internal steps were taken by IDASolve, the returned values of tret,yret, and ypret correspond to the farthest point reached in the integration. On all other error returns, these values are left unchanged from the previous IDASolve return.

5.5.6 Optional input functions

IDA provides an extensive list of functions that can be used to change various optional input parameters that control the behavior of the IDA solver from their default values. Table 5.1 lists all optional input functions in IDA which are then described in detail in the remainder of this section. For the most casual use of IDA, the reader can skip to §5.6.

We note that, on error return, all these functions also send an error message to the error handler function. We also note that all error return values are negative, so a test flag < 0 will catch any error.

Table 5.1: Optional inputs for IDA, IDADENSE, IDABAND, and IDASPILS

Optional input	Function name	Default
IDA main solver		
Error handler function	IDASetErrHandlerFn	internal fn.
Pointer to an error file	IDASetErrFile	stderr
Data for residual function	IDASetRdata	NULL
Maximum order for BDF method	IDASetMaxOrd	5
Maximum no. of internal steps before t_{out}	IDASetMaxNumSteps	500
Initial step size	IDASetInitStep	estimated
Maximum absolute step size	IDASetMaxStep	∞
Value of t_{stop}	IDASetStopTime	∞
Maximum no. of error test failures	IDASetMaxErrTestFails	10
Maximum no. of nonlinear iterations	IDASetMaxNonlinIters	4
Maximum no. of convergence failures	IDASetMaxConvFails	10
Maximum no. of error test failures	IDASetMaxErrTestFails	7
Coeff. in the nonlinear convergence test	IDASetNonlinConvCoef	0.33
Suppress alg. vars. from error test	IDASetSuppressAlg	FALSE
Variable types (differential/algebraic)	IDASetId	NULL
Inequality constraints on solution	IDASetConstraints	NULL
Integration tolerances	IDASetTolerances	none
IDA initial conditions calculation		
Coeff. in the nonlinear convergence test	IDASetNonlinConvCoefIC	0.0033
Maximum no. of steps	IDASetMaxNumStepsIC	5
Maximum no. of Jacobian/precond. evals.	IDASetMaxNumJacsIC	4
Maximum no. of Newton iterations	IDASetMaxNumItersIC	10
Turn off linesearch	IDASetLineSearchOffIC	FALSE
Lower bound on Newton step	IDASetStepToleranceIC	uround$^{2/3}$
IDADENSE linear solver		
Dense Jacobian function and data	IDADenseSetJacFn	DQ, NULL
IDABAND linear solver		
Band Jacobian function and data	IDABandSetJacFn	DQ, NULL
IDASPILS linear solvers		
Preconditioner functions and data	IDASpilsSetPreconditioner	all NULL
Jacobian-times-vector function and data	IDASpilsSetJacTimesVecFn	DQ, NULL
Factor in linear convergence test	IDASpilsSetEpsLin	0.05
Factor in DQ increment calculation	IDASpilsSetIncrementFactor	1.0
Maximum no. of restarts (IDASPGMR)	IDASpilsSetMaxRestarts	5
Type of Gram-Schmidt orthogonalization [(a)]	IDASpilsSetGSType	classical GS
Maximum Krylov subspace size[(b)]	IDASpilsSetMaxl	5

[(a)] Only for IDASPGMR
[(b)] Only for IDASPBCG and IDASPTFQMR

5.5.6.1 Main solver optional input functions

The calls listed here can be executed in any order.
However, if IDASetErrHandlerFn or IDASetErrFile are to be called, that call should be first, in order to take effect for any later error message.

IDASetErrHandlerFn

Call `flag = IDASetErrHandlerFn(ida_mem, ehfun, eh_data);`

Description The function IDASetErrHandlerFn specifies the optional user-defined function to be used in handling error messages.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`ehfun` (`IDAErrHandlerFn`) is the C error handler function (see §5.6.2).
`eh_data` (`void *`) pointer to user data passed to `ehfun` every time it is called.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The function `ehfun` and data pointer `eh_data` have been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default internal error handler function directs error messages to the file specified by the file pointer `errfp` (see IDASetErrFile below).

Error messages indicating that the IDA solver memory is `NULL` will always be directed to `stderr`.

IDASetErrFile

Call `flag = IDASetErrFile(ida_mem, errfp);`

Description The function IDASetErrFile specifies the pointer to the file where all IDA messages should be directed in case the default IDA error handler function is used.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`errfp` (`FILE *`) pointer to output file.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value for `errfp` is `stderr`.

Passing a value `NULL` disables all future error message output (except for the case in which the IDA memory pointer is `NULL`).

If IDASetErrFile is to be called, it should be called before any other optional input functions, in order to take effect for any later error message.

IDASetRdata

Call `flag = IDASetRdata(ida_mem, res_data);`

Description The function IDASetRdata specifies the user data block `res_data` and attaches it to the main IDA memory block.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`res_data` (`void *`) pointer to the user data.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes If `res_data` is not specified, a `NULL` pointer is passed to all user functions that have it as an argument.

`IDASetMaxOrd`

Call `flag = IDASetMaxOrd(ida_mem, maxord);`

Description The function `IDASetMaxOrd` specifies the maximum order of the linear multistep method.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxord` (`int`) value of the maximum method order.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` The specified value `maxord` is negative, or larger than its previous value.

Notes The default value is 5. Since `maxord` affects the memory requirements for the internal IDA memory block, its value can not be increased past its previous value.

`IDASetMaxNumSteps`

Call `flag = IDASetMaxNumSteps(ida_mem, mxsteps);`

Description The function `IDASetMaxNumSteps` specifies the maximum number of steps to be taken by the solver in its attempt to reach the next output time.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`mxsteps` (`long int`) maximum allowed number of steps.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` `mxsteps` is non-positive.

Notes Passing `mxsteps`$= 0$ results in IDA using the default value (500).

`IDASetInitStep`

Call `flag = IDASetInitStep(ida_mem, hin);`

Description The function `IDASetInitStep` specifies the initial step size.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`hin` (`realtype`) value of the initial step size.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes By default, IDA estimates the initial step as the solution of $\|hy'\|_{\mathrm{WRMS}} = 1/2$, with an added restriction that $|h| \leq .001|$`tout - t0`$|$.

`IDASetMaxStep`

Call `flag = IDASetMaxStep(ida_mem, hmax);`

Description The function `IDASetMaxStep` specifies the maximum absolute value of the step size.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`hmax` (`realtype`) maximum absolute value of the step size.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_ILL_INPUT` Either `hmax` is not positive or it is smaller than the minimum allowable step.

Notes Pass `hmax`$= 0$ to obtain the default value ∞.

`IDASetStopTime`

Call `flag = IDASetStopTime(ida_mem, tstop);`

Description The function `IDASetStopTime` specifies the value of the independent variable t past which the solution is not to proceed.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`tstop` (`realtype`) value of the independent variable past which the solution should not proceed.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default, if this routine is not called, is that no stop time is imposed.

`IDASetMaxErrTestFails`

Call `flag = IDASetMaxErrTestFails(ida_mem, maxnef);`

Description The function `IDASetMaxErrTestFails` specifies the maximum number of error test failures in attempting one step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxnef` (`int`) maximum number of error test failures allowed on one step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 7.

`IDASetMaxNonlinIters`

Call `flag = IDASetMaxNonlinIters(ida_mem, maxcor);`

Description The function `IDASetMaxNonlinIters` specifies the maximum number of nonlinear solver iterations at one step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxcor` (`int`) maximum number of nonlinear solver iterations allowed on one step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 3.

`IDASetMaxConvFails`

Call `flag = IDASetMaxConvFails(ida_mem, maxncf);`

Description The function `IDASetMaxConvFails` specifies the maximum number of nonlinear solver convergence failures at one step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxncf` (`int`) maximum number of allowable nonlinear solver convergence failures on one step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 10.

`IDASetNonlinConvCoef`

Call `flag = IDASetNonlinConvCoef(ida_mem, nlscoef);`

Description The function `IDASetNonlinConvCoef` specifies the safety factor in the nonlinear convergence test; see Chapter 3, Eq. (3.7).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`nlscoef` (`realtype`) coefficient in nonlinear convergence test.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 0.33.

`IDASetSuppressAlg`

Call `flag = IDASetSuppressAlg(ida_mem, suppressalg);`

Description The function `IDASetSuppressAlg` indicates whether or not to suppress algebraic variables in the local error test.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`suppresslag` (`booleantype`) indicates whether to suppress (`TRUE`) or not (`FALSE`) the algebraic variables in the local error test.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is `FALSE`.

If `suppresslag`=`TRUE` is selected, then the `id` vector must be set (through `IDASetId`) to specify the algebraic components.

`IDASetId`

Call `flag = IDASetId(ida_mem, id);`

Description The function `IDASetId` specifies algebraic/differential components in the y vector.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`id` (`N_Vector`) state vector. A value of 1.0 indicates a differential variable, while 0.0 indicates an algebraic variable.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The vector `id` is required if the algebraic variables are to be suppressed from the local error test (see `IDASetSuppressAlg`) or if `IDACalcIC` is to be called with `icopt` = `IDA_YA_YDP_INIT` (see §5.5.4).

`IDASetConstraints`

Call `flag = IDASetConstraints(ida_mem, constraints);`

Description The function `IDASetConstraints` specifies a vector defining inequality constraints for each component of the solution vector y.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`constraints` (`N_Vector`) vector of constraint flags. If `constraints[i]` is

- 0.0 then no constraint is imposed on y_i.
- 1.0 then y_i will be constrained to be $y_i \geq 0.0$.
- −1.0 then y_i will be constrained to be $y_i \leq 0.0$.
- 2.0 then y_i will be constrained to be $y_i > 0.0$.
- −2.0 then y_i will be constrained to be $y_i < 0.0$.

Return value The return value `flag` (of type `int`) is one of

- `IDA_SUCCESS` The optional value has been successfuly set.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDA_ILL_INPUT` The constraints vector contains illegal values.

Notes The presence of a non-`NULL` constraints vector that is not 0.0 in all components will cause constraint checking to be performed.

`IDASetTolerances`

Call `flag = IDASetTolerances(ida_mem, itol, reltol, abstol);`

Description The function `IDASetTolerances` resets the integration tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`itol` (`int`) is either `IDA_SS` or `IDA_SV`, where `itol`=`IDA_SS` indicates scalar relative error tolerance and scalar absolute error tolerance, while `itol`=`IDA_SV` indicates scalar relative error tolerance and vector absolute error tolerance. The latter choice is important when the absolute error tolerance needs to be different for each component of the DAE.

`reltol` (`realtype`) is the relative error tolerance.

`abstol` (`void *`) is a pointer to the absolute error tolerance. If `itol`=`IDA_SS`, `abstol` must be a pointer to a `realtype` variable. If `itol` = `IDA_SV`, `abstol` must be an `N_Vector` variable.

Return value The return value `flag` (of type `int`) is one of

- `IDA_SUCCESS` The tolerances have been successfully set.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDA_ILL_INPUT` An input argument has an illegal value.

Notes The integration tolerances are initially specified in the call to `IDAMalloc` (see §5.5.1). This function call to `IDASetTolerances` is needed only if the tolerances are being changed from their values between successive calls to `IDASolve`.

It is the user's responsibility to provide compatible `itol` and `abstol` arguments.

It is illegal to call `IDASetTolerances` before a call to `IDAMalloc`.

`IDASetEwtFn`

Call `flag = IDASetEwtFn(ida_mem, efun, edata);`

Description The function `IDASetEwtFn` specifies the user-defined function that sets the multiplicative error weights W_i for use in the weighted RMS norm, which are normally defined by Eq. (3.6).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`efun` (`IDAEwtFn`) is the C function which defines the `ewt` vector (see §5.6.3).
`edata` (`void *`) pointer to user data passed to `efun` every time it is called.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The function `efun` and data pointer `edata` have been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes This function can be called between successive calls to `IDASolve`.

If not needed, pass `NULL` for `edata`.

It is illegal to call `IDASetEwtFn` before a call to `IDAMalloc`.

5.5.6.2 Initial condition calculation optional input functions

The following functions can be called to set optional inputs to control the initial condition calculations.

`IDASetNonlinConvCoefIC`

Call `flag = IDASetNonlinConvCoefIC(ida_mem, epiccon);`

Description The function `IDASetNonlinConvCoefIC` specifies the positive constant in the Newton iteration convergence test within the initial condition calculation.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`epiccon` (`realtype`) coefficient in the Newton convergence test.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` The `epiccon` factor is negative (illegal).

Notes The default value is $0.01 \cdot 0.33$.

This test uses a weighted RMS norm (with weights defined by the tolerances). For new initial value vectors y and y' to be accepted, the norm of $J^{-1}F(t_0, y, y')$ must be $\leq$ `epiccon`, where J is the system Jacobian.

`IDASetMaxNumStepsIC`

Call `flag = IDASetMaxNumStepsIC(ida_mem, maxnh);`

Description The function `IDASetMaxNumStepsIC` specifies the maximum number of steps allowed when `icopt`=`IDA_YA_YDP_INIT` in `IDACalcIC`, where h appears in the system Jacobian, $J = \partial F/\partial y + (1/h)\partial F/\partial y'$.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxnh` (`int`) maximum allowed number of values for h.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` `maxnh` is non-positive.

Notes The default value is 5.

IDASetMaxNumJacsIC

Call `flag = IDASetMaxNumJacsIC(ida_mem, maxnj);`

Description The function `IDASetMaxNumJacsIC` specifies the maximum number of the approximate Jacobian or preconditioner evaluations allowed when the Newton iteration appears to be slowly converging.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxnj` (`int`) maximum allowed number of Jacobian or preconditioner evaluations.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` `maxnj` is non-positive.

Notes The default value is 4.

IDASetMaxNumItersIC

Call `flag = IDASetMaxNumItersIC(ida_mem, maxnit);`

Description The function `IDASetMaxNumItersIC` specifies the maximum number of Newton iterations allowed in any one attempt to solve the initial conditions calculation problem.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxnit` (`int`) maximum number of Newton iterations.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` `maxnit` is non-positive.

Notes The default value is 10.

IDASetLineSearchOffIC

Call `flag = IDASetLineSearchOffIC(ida_mem, lsoff);`

Description The function `IDASetLineSearchOffIC` specifies whether to turn on or off the linesearch algorithm.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`lsoff` (`booleantype`) a flag to turn off (`TRUE`) or keep (`FALSE`) the linesearch algorithm.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is `FALSE`.

IDASetStepToleranceIC

Call `flag = IDASetStepToleranceIC(ida_mem, steptol);`

Description The function `IDASetStepToleranceIC` specifies a positive lower bound on the Newton step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`steptol` (`int`) Newton step tolerance.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfuly set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	The `steptol` tolerance is negative (illegal).

Notes The default value is (unit roundoff)$^{2/3}$.

5.5.6.3 Linear solver optional input functions

The linear solver modules allow for various optional inputs, which are described here.

5.5.6.4 Dense linear solver

The IDADENSE solver needs a function to compute a dense approximation to the Jacobian matrix $J(t, y, y')$. This function must be of type `IDADenseJacFn`. The user can supply his/her own dense Jacobian function, or use the default difference quotient function `IDADenseDQJac` that comes with the IDADENSE solver. To specify a user-supplied Jacobian function `djac` and associated user data `jac_data`, IDADENSE provides the function `IDADenseSetJacFn`. The IDADENSE solver passes the pointer `jac_data` to its dense Jacobian function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer `jac_data` may be identical to `res_data`, if the latter was specified through `IDASetFdata`.

`IDADenseSetJacFn`

Call `flag = IDADenseSetJacFn(ida_mem, djac, jac_data);`

Description The function `IDADenseSetJacFn` specifies the dense Jacobian approximation function to be used and the pointer to user data.

Arguments

`ida_mem`	(`void *`) pointer to the IDA memory block.
`djac`	(`IDADenseJacFn`) user-defined dense Jacobian approximation function.
`jac_data`	(`void *`) pointer to the user-defined data structure.

Return value The return value `flag` (of type `int`) is one of

`IDADENSE_SUCCESS`	The optional value has been successfully set.
`IDADENSE_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADENSE_LMEM_NULL`	The IDADENSE linear solver has not been initialized.

Notes By default, IDADENSE uses the difference quotient function `IDADenseDQJac`. If `NULL` is passed to `djac`, this default function is used.

The function type `IDADenseJacFn` is described in §5.6.4.

5.5.6.5 Band linear solver

The IDABAND solver needs a function to compute a banded approximation to the Jacobian matrix $J(t, y, y')$. This function must be of type `IDABandJacFn`. The user can supply his/her own banded Jacobian approximation function, or use the default difference quotient function `IDABandDQJac` that comes with the IDABAND solver. To specify a user-supplied Jacobian function `bjac` and associated user data `jac_data`, IDABAND provides the function `IDABandSetJacFn`. The IDABAND solver passes the pointer `jac_data` to its banded Jacobian approximation function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer `jac_data` may be identical to `res_data`, if the latter was specified through `IDAodeSetFdata`.

`IDABandSetJacFn`

Call `flag = IDABandSetJacFn(ida_mem, bjac, jac_data);`

Description The function `IDABandSetJacFn` specifies the banded Jacobian approximation function to be used and the pointer to user data.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `bjac` (`IDABandJacFn`) user-defined banded Jacobian approximation function.
- `jac_data` (`void *`) pointer to the user-defined data structure.

Return value The return value `flag` (of type `int`) is one of
- `IDABAND_SUCCESS` The optional value has been successfully set.
- `IDABAND_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDABAND_LMEM_NULL` The IDABAND linear solver has not been initialized.

Notes By default, IDABAND uses the difference quotient function `IDABandDQJac`. If `NULL` is passed to `bjac`, this default function is used.

The function type `IDABandJacFn` is described in §5.6.5.

5.5.6.6 SPGMR Linear solver

If preconditioning is to be done with one of the IDASPILS linear solvers, then the user must supply a preconditioner solve function and specify its name through a call to `IDASpilsSetPreconditioner`. The evaluation and preprocessing of any Jacobian-related data needed by the user's preconditioner solve function is done in the optional user-supplied function `psetup`. Both of these functions are fully specified in §5.6. If used, the name of the `psetup` function should be specified in the call to `IDASpilsSetPreconditioner`.

Optionally, the pointer `p_data` received through `IDASpilsSetPreconditioner` is passed to the preconditioner `psetup` and `psolve` functions. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied preconditioner functions without using global data in the program. The pointer `p_data` may be identical to `res_data`, if the latter was specified through `IDASetRdata`.

The IDASPILS solvers require a function to compute an approximation to the product between the Jacobian matrix $J(t, y)$ and a vector v. The user can supply his/her own Jacobian-times-vector approximation function, or use the difference quotient function `IDASpilsDQJtimes` that comes with the IDASPILS solvers. A user-defined Jacobian-vector function must be of type `IDASpilsJacTimesVecFn` and can be specified through a call to `IDASpilsSetJacTimesVecFn` (see §5.6.6 for specification details). As with the preconditioner user data structure `p_data`, the user can also specify in the call to `IDASpilsSetJacTimesVecFn`, a pointer to a user-defined data structure, `jac_data`, which the IDASPILS solver passes to the Jacobian-times-vector function `jtimes` each time it is called. The pointer `jac_data` may be identical to `p_data` and/or `res_data`.

`IDASpilsSetPreconditioner`

Call `flag = IDASpilsSetPreconditioner(ida_mem, psetup, psolve, p_data);`

Description The function `IDASpilsSetPreconditioner` specifies the preconditioner setup and solve functions and the pointer to user data.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `psetup` (`IDASpilsPrecSetupFn`) user-defined preconditioner setup function.
- `psolve` (`IDASpilsPrecSolveFn`) user-defined preconditioner solve function.
- `p_data` (`void *`) pointer to the user-defined data structure.

Return value The return value `flag` (of type `int`) is one of
- `IDASPILS_SUCCESS` The optional value has been successfully set.
- `IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_LMEM_NULL` The IDASPILS linear solver has not been initialized.

Notes The function type `IDASpilsPrecSolveFn` is described in §5.6.7. The function type `IDASpilsPrecSetupFn` is described in §5.6.8.

`IDASpilsSetJacTimesVecFn`

Call `flag = IDASpilsSetJacTimesVecFn(ida_mem, jtimes, jac_data);`

Description The function `IDASpilsSetJacTimesFn` specifies the Jacobian-vector function to be used and the pointer to user data.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`jtimes` (`IDASpilsJacTimesVecFn`) user-defined Jacobian-vector product function.
`jac_data` (`void *`) pointer to the user-defined data structure.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional value has been successfully set.
`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL` The IDASPILS linear solver has not been initialized.

Notes By default, the IDASPILS solvers use the difference quotient function `IDASpilsDQJtimes`. If `NULL` is passed to `jtimes`, this default function is used.

The function type `IDASpilsJacTimesVecFn` is described in §5.6.6.

`IDASpilsSetGSType`

Call `flag = IDASpilsSetGSType(ida_mem, gstype);`

Description The function `IDASpilsSetGSType` specifies the Gram-Schmidt orthogonalization to be used. This must be one of the enumeration constants `MODIFIED_GS` or `CLASSICAL_GS`. These correspond to using modified Gram-Schmidt and classical Gram-Schmidt, respectively.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`gstype` (`int`) type of Gram-Schmidt orthogonalization.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional value has been successfuly set.
`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL` The IDASPILS linear solver has not been initialized.
`IDASPILS_ILL_INPUT` The Gram-Schmidt orthogonalization type `gstype` is not valid.

Notes The default value is `MODIFIED_GS`.

This option is available only for the IDASPGMR linear solver.

`IDASpilsSetMaxRestarts`

Call `flag = IDASpilsSetMaxRestarts(ida_mem, maxrs);`

Description The function `IDASpilsSetMaxRestarts` specifies the maximum number of restarts to be used in the GMRES algorithm.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxrs` (`int`) maximum number of restarts.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional value has been successfuly set.
`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT The maxrs argument is negative.

Notes The default value is 5. Pass maxrs = 0 to specify no restarts.

This option is available only for the IDASPGMR linear solver.

IDASpilsSetEpsLin

Call flag = IDASpilsSetEpsLin(ida_mem, eplifac);

Description The function IDASpilsSetEpsLin specifies the factor by which the GMRES convergence test constant is reduced from the Newton iteration test constant. (See §3).

Arguments ida_mem (void *) pointer to the IDA memory block.
eplifac (realtype)

Return value The return value flag (of type int) is one of

IDASPILS_SUCCESS The optional value has been successfuly set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT The factor eplifac is negative.

Notes The default value is 0.05.

Passing a value eplifac= 0.0 also indicates using the default value.

IDASpilsSetIncrementFactor

Call flag = IDASpilsSetIncrementFactor(ida_mem, dqincfac);

Description The function IDASpilsSetIncrementFactor specifies a factor in the increments to y used in the difference quotient approximations to the Jacobian-vector products. (See §3).

Arguments ida_mem (void *) pointer to the IDA memory block.
dqincfac (realtype) difference quotient increment factor.

Return value The return value flag (of type int) is one of

IDASPILS_SUCCESS The optional value has been successfuly set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT The increment factor was non-positive.

Notes The default value is dqincfac = 1.0.

IDASpbcgSetMaxl

Call flag = IDASpbcgSetMaxl(ida_mem, maxl);

Description The function IDASpbcgSetMaxl specifies maximum of the Krylov subspace dimension for the Bi-CGStab method.

Arguments ida_mem (void *) pointer to the IDA memory block.
maxl (int) maximum dimension of the Krylov subspace.

Return value The return value flag (of type int) is one of

IDASPILS_SUCCESS The optional value has been successfuly set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.

Notes The default value is 5. Passing maxl = 0 also results in the default value.

This option is available only for the IDASPBCG and IDASPTFQMR linear solvers.

5.5.7 Interpolated output function

An optional function `IDAGetSolution` is available to obtain additional output values. This function must be called after a successful return from `IDASolve` and provides interpolated values of y and y' for any value of t in the last internal step taken by IDA.

The call to the `IDAGetSolution` function has the following form:

`IDAGetSolution`

Call `flag = IDAGetSolution(ida_mem, t, yret, ypret);`

Description The function `IDAGetSolution` computes the interpolated values of y and y' for any value of t in the last internal step taken by IDA. The value of t must satisfy $t_n - h_u \le t \le t_n$, where t_n denotes the current internal time reached, and h_u is the last internal step size used successfully.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `t` (`realtype`)
- `yret` (`N_Vector`) vector containing the interpolated $y(t)$.
- `ypret` (`N_Vector`) vector containing the interpolated $y'(t)$.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` `IDAGetSolution` succeeded.
- `IDA_MEM_NULL` The `ida_mem` argument was `NULL`.
- `IDA_BAD_T` `t` is not in the interval $[t_n - h_u, t_n]$.

Notes It is only legal to call the function `IDAGetSolution` after a successful return from `IDASolve`. See `IDAGetCurrentTime` and `IDAGetLastStep` for access to t_n and h_u.

5.5.8 Optional output functions

IDA provides an extensive list of functions that can be used to obtain solver performance information. Table 5.2 lists all optional output functions in IDA, which are then described in detail in the remainder of this section.

5.5.8.1 Main solver optional output functions

IDA provides several user-callable functions that can be used to obtain different quantities that may be of interest to the user, such as solver workspace requirements, solver performance statistics, as well as additional data from the IDA memory block (a suggested tolerance scaling factor, the error weight vector, and the vector of estimated local errors). Also provided are functions to extract statistics related to the performance of the IDA nonlinear solver being used. As a convenience, additional extraction functions provide the optional outputs in groups. These optional output functions are described next.

`IDAGetWorkSpace`

Call `flag = IDAGetWorkSpace(ida_mem, &lenrw, &leniw);`

Description The function `IDAGetWorkSpace` returns the IDA real and integer workspace sizes.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `lenrw` (`long int`) number of real values in the IDA workspace.
- `leniw` (`long int`) number of integer values in the IDA workspace.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The optional output value has been successfuly set.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Table 5.2: Optional outputs from IDA, IDADENSE, IDABAND, and IDASPILS

Optional output	Function name
IDA main solver	
Size of IDA real and integer workspace	IDAGetWorkSpace
Cumulative number of internal steps	IDAGetNumSteps
No. of calls to residual function	IDAGetNumResEvals
No. of calls to linear solver setup function	IDAGetNumLinSolvSetups
No. of local error test failures that have occurred	IDAGetNumErrTestFails
Order used during the last step	IDAGetLastOrder
Order to be attempted on the next step	IDAGetCurrentOrder
Order reductions due to stability limit detection	IDAGetNumStabLimOrderReds
Actual initial step size used	IDAGetActualInitStep
Step size used for the last step	IDAGetLastStep
Step size to be attempted on the next step	IDAGetCurrentStep
Current internal time reached by the solver	IDAGetCurrentTime
Suggested factor for tolerance scaling	IDAGetTolScaleFactor
Error weight vector for state variables	IDAGetErrWeights
Estimated local errors	IDAGetEstLocalErrors
No. of nonlinear solver iterations	IDAGetNumNonlinSolvIters
No. of nonlinear convergence failures	IDAGetNumNonlinSolvConvFails
Array showing roots found	IDAGetRootInfo
No. of calls to user root function	IDAGetNumGEvals
Name of constant associated with a return flag	IDAGetReturnFlagName
IDA initial conditions calculation	
Number of backtrack operations	IDAGatNumBacktrackops
Corrected initial conditions	IDAGetConsistentIC
IDADENSE linear solver	
Size of IDADENSE real and integer workspace	IDADenseGetWorkSpace
No. of Jacobian evaluations	IDADenseGetNumJacEvals
No. of residual calls for finite diff. Jacobian evals.	IDADenseGetNumResEvals
Last return from a IDADENSE function	IDADenseGetLastFlag
Name of constant associated with a return flag	IDADenseGetReturnFlagName
IDABAND linear solver	
Size of IDABAND real and integer workspace	IDABandGetWorkSpace
No. of Jacobian evaluations	IDABandGetNumJacEvals
No. of residual calls for finite diff. Jacobian evals.	IDABandGetNumResEvals
Last return from a IDABAND function	IDABandGetLastFlag
Name of constant associated with a return flag	IDABandGetReturnFlagName
IDASPILS linear solvers	
Size of real and integer workspace	IDASpilsGetWorkSpace
No. of linear iterations	IDASpilsGetNumLinIters
No. of linear convergence failures	IDASpilsGetNumConvFails
No. of preconditioner evaluations	IDASpilsGetNumPrecEvals
No. of preconditioner solves	IDASpilsGetNumPrecSolves
No. of Jacobian-vector product evaluations	IDASpilsGetNumJtimesEvals
No. of residual calls for finite diff. Jacobian-vector evals.	IDASpilsGetNumResEvals
Last return from a linear solver function	IDASpilsGetLastFlag
Name of constant associated with a return flag	IDASpilsGetReturnFlagName

Notes In terms of the problem size N, the maximum method order `maxord`, and the number `nrtfn` of root functions (see §5.7), the actual size of the real workspace, in `realtype` words, is given by the following:

- base value: `lenrw` $= 55 + (m + 6) * N_r + 3*$`nrtfn`;
- with `itol = IDA_SV`: `lenrw` $=$ `lenrw` $+N_r$;
- with constraint checking (see `IDASetConstraints`): `lenrw` $=$ `lenrw` $+N_r$;
- with `id` specified (see `IDASetId`): `lenrw` $=$ `lenrw` $+N_r$;

where $m = \max($`maxord`$, 3)$, and N_r is the number of real words in one `N_Vector` ($\approx N$).

The size of the integer workspace (without distinction between `int` and `long int` words) is given by:

- base value: `leniw` $= 38 + (m + 6) * N_i$ $+$ `nrtfn`;
- with `itol = IDA_SV`: `leniw` $=$ `leniw` $+N_i$;
- with constraint checking: `lenrw` $=$ `lenrw` $+N_i$;
- with `id` specified: `lenrw` $=$ `lenrw` $+N_i$;

where N_i is the number of integer words in one `N_Vector` ($= 1$ for NVECTOR_SERIAL and 2*`npes` for NVECTOR_PARALLEL on `npes` processors).

For the default value of `maxord`, with no rootfinding, no `id`, no constraints, and with `itol` $\neq$ `IDA_SV`, these lengths are given roughly by: `lenrw` $= 55 + 11N$, `leniw` $= 38$.

`IDAGetNumSteps`

Call `flag = IDAGetNumSteps(ida_mem, &nsteps);`

Description The function `IDAGetNumSteps` returns the cumulative number of internal steps taken by the solver (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nsteps` (`long int`) number of steps taken by IDA.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetNumResEvals`

Call `flag = IDAGetNumResEvals(ida_mem, &nrevals);`

Description The function `IDAGetNumResEvals` returns the number of calls to the user's residual evaluation function.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nrevals` (`long int`) number of calls to the user's `res` function.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The `nrevals` value returned by `IDAGetNumResEvals` does not account for calls made to `res` from a linear solver or preconditioner module.

`IDAGetNumLinSolvSetups`

Call `flag = IDAGetNumLinSolvSetups(ida_mem, &nlinsetups);`

Description The function `IDAGetNumLinSolvSetups` returns the cumulative number of calls made to the linear solver's setup function (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nlinsetups` (`long int`) number of calls made to the linear solver setup function.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetNumErrTestFails`

Call `flag = IDAGetNumErrTestFails(ida_mem, &netfails);`

Description The function `IDAGetNumErrTestFails` returns the cumulative number of local error test failures that have occurred (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`netfails` (`long int`) number of error test failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetLastOrder`

Call `flag = IDAGetLastOrder(ida_mem, &qlast);`

Description The function `IDAGetLastOrder` returns the integration method order used during the last internal step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`qlast` (`int`) method order used on the last internal step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetCurrentOrder`

Call `flag = IDAGetCurrentOrder(ida_mem, &qcur);`

Description The function `IDAGetCurrentOrder` returns the integration method order to be used on the next internal step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`qcur` (`int`) method order to be used on the next internal step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetLastStep`

Call `flag = IDAGetLastStep(ida_mem, &hlast);`

Description The function `IDAGetLastStep` returns the integration step size taken on the last internal step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`hlast` (`realtype`) step size taken on the last internal step.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetCurrentStep`

Call `flag = IDAGetCurrentStep(ida_mem, &hcur);`

Description The function `IDAGetCurrentStep` returns the integration step size to be attempted on the next internal step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`hcur` (`realtype`) step size to be attempted on the next internal step.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetActualInitStep`

Call `flag = IDAGetActualInitStep(ida_mem, &hinused);`

Description The function `IDAGetActualInitStep` returns the value of the integration step size used on the first step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`hinused` (`realtype`) actual value of initial step size.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes Even if the value of the initial integration step size was specified by the user through a call to `IDASetInitStep`, this value might have been changed by IDA to ensure that the step size is within the prescribed bounds ($h_{\min} \le h_0 \le h_{\max}$), or to meet the local error test.

`IDAGetCurrentTime`

Call `flag = IDAGetCurrentTime(ida_mem, &tcur);`

Description The function `IDAGetCurrentTime` returns the current internal time reached by the solver.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`tcur` (`realtype`) current internal time reached.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetTolScaleFactor`

Call `flag = IDAGetTolScaleFactor(ida_mem, &tolsfac);`

Description The function `IDAGetTolScaleFactor` returns a suggested factor by which the user's tolerances should be scaled when too much accuracy has been requested for some internal step.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`tolsfac` (`realtype`) suggested scaling factor for user tolerances.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetErrWeights`

Call `flag = IDAGetErrWeights(ida_mem, eweight);`

Description The function `IDAGetErrWeights` returns the solution error weights at the current time. These are the W_i given by Eq. (3.6) (or by the user's `IDAEwtFn`).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`eweight` (`N_Vector`) solution error weights at the current time.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The user must allocate space for `eweight`.

`IDAGetEstLocalErrors`

Call `flag = IDAGetEstLocalErrors(ida_mem, ele);`

Description The function `IDAGetEstLocalErrors` returns the estimated local errors.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`eweight` (`N_Vector`) estimated local errors at the current time.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The user must allocate space for `ele`.
The values returned in `ele` are only valid if `IDASolve` returned a positive value.

The `ele` vector, togther with the `eweight` vector from `IDAGetErrWeights`, can be used to determine how the various components of the system contributed to the estimated local error test. Specifically, that error test uses the RMS norm of a vector whose components are the products of the components of the two vectors. Thus, for example, if there were recent error test failures, the components causing the failures are those with largest values for the products, denoted loosely as `eweight[i]*ele[i]`.

`IDAGetIntegratorStats`

Call
```
flag = IDAGetIntegratorStats(ida_mem, &nsteps, &nrevals, &nlinsetups,
                             &netfails, &qlast, &qcur, &hinused,
                             &hlast, &hcur, &tcur);
```

Description The function `IDAGetIntegratorStats` returns the IDA integrator statistics as a group.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`nsteps`	(`long int`) cumulative number of steps taken by IDA.
`nrevals`	(`long int`) cumulative number of calls to the user's `res` function.
`nlinsetups`	(`long int`) cumulative number of calls made to the linear solver setup function.
`netfails`	(`long int`) cumulative number of error test failures.
`qlast`	(`int`) method order used on the last internal step.
`qcur`	(`int`) method order to be used on the next internal step.
`hinused`	(`realtype`) actual value of initial step size.
`hlast`	(`realtype`) step size taken on the last internal step.
`hcur`	(`realtype`) step size to be attempted on the next internal step.
`tcur`	(`realtype`) current internal time reached.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	the optional output values have been successfuly set.
`IDA_MEM_NULL`	the `ida_mem` pointer is `NULL`.

`IDAGetNumNonlinSolvIters`

Call `flag = IDAGetNumNonlinSolvIters(ida_mem, &nniters);`

Description The function `IDAGetNumNonlinSolvIters` returns the cumulative number of nonlinear (functional or Newton) iterations performed.

Arguments

`ida_mem`	(`void *`) pointer to the IDA memory block.
`nniters`	(`long int`) number of nonlinear iterations performed.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfuly set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetNumNonlinSolvConvFails`

Call `flag = IDAGetNumNonlinSolvConvFails(ida_mem, &nncfails);`

Description The function `IDAGetNumNonlinSolvConvFails` returns the cumulative number of nonlinear convergence failures that have occurred.

Arguments

`ida_mem`	(`void *`) pointer to the IDA memory block.
`nncfails`	(`long int`) number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfuly set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetNonlinSolvStats`

Call `flag = IDAGetNonlinSolvStats(ida_mem, &nniters, &nncfails);`

Description The function `IDAGetNonlinSolvStats` returns the IDA nonlinear solver statistics as a group.

Arguments

`ida_mem`	(`void *`) pointer to the IDA memory block.
`nniters`	(`long int`) cumulative number of nonlinear iterations performed.
`nncfails`	(`long int`) cumulative number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfuly set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetReturnFlagName`

Call `name = IDAGetReturnFlagName(flag);`

Description The function `IDAGetReturnFlagName` returns the name of the IDA constant corresponding to `flag`.

Arguments The only argument, of type `int` is a return flag from a IDA function.

Return value The return value is a string containing the name of the corresponding constant.

5.5.8.2 Initial condition calculation optional output functions

`IDAGetNumBcktrackOps`

Call `flag = IDAGetNumBacktrackOps(ida_mem, &nbacktr);`

Description The function `IDAGetNumBacktrackOps` returns the number of backtrack operations done in the linesearch algorithm in `IDACalcIC`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nbacktr` (`long int`) the cumulative number of backtrack operations.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetConsistentIC`

Call `flag = IDAGetConsistentIC(ida_mem, yy0_mod, yp0_mod);`

Description The function `IDAGetConsistentIC` returns the corrected initial conditions calculated by `IDACalcIC`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`yy0_mod` (`N_Vector`) consistent solution vector.
`yp0_mod` (`N_Vector`) consistent derivative vector.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_ILL_INPUT` The fucntion was not called before the first call to `IDASolve`.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes If the consistent solution vector or consistent derivative vector is not desired, pass `NULL` for the corresponding argument.

The user must allocate space for `yy0_mod` and `yp0_mod` (if not `NULL`).

5.5.8.3 Linear solver optional output functions

For each of the linear system solver modules, there are various optional outputs that describe the performance of the module. The functions available to access these are described below. Where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix `LS` (for Linear Solver) has been added here (e.g. `lenrwLS`).

5.5.8.4 Dense linear solver

The following optional outputs are available from the IDADENSE module: workspace requirements, number of calls to the Jacobian routine, number of calls to the residual routine for finite-difference Jacobian approximation, and last return value from a IDADENSE function.

`IDADenseGetWorkSpace`

Call `flag = IDADenseGetWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDADenseGetWorkSpace` returns the sizes of the IDADENSE real and integer workspaces.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`lenrwLS` (`long int`) the number of real values in the IDADENSE workspace.
`leniwLS` (`long int`) the number of integer values in the IDADENSE workspace.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfuly set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_MEM_NULL` The IDADENSE linear solver has not been initialized.

Notes In terms of the problem size N, the actual size of the real workspace is $2N^2$ `realtype` words. The actual size of the integer workspace is N integer words.

`IDADenseGetNumJacEvals`

Call `flag = IDADenseGetNumJacEvals(ida_mem, &njevals);`

Description The function `IDADenseGetNumJacEvals` returns the cumulative number of calls to the dense Jacobian approximation function.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`njevals` (`long int`) the cumulative number of calls to the Jacobian function (total so far).

Return value The return value `flag` (of type `int`) is one of
`IDADENSE_SUCCESS` The optional output value has been successfuly set.
`IDADENSE_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDADENSE_LMEM_NULL` The IDADENSE linear solver has not been initialized.

`IDADenseGetNumResEvals`

Call `flag = IDADenseGetNumResEvals(ida_mem, &nrevalsLS);`

Description The function `IDADenseGetNumResEvals` returns the cumulative number of calls to the user residual function due to the finite difference dense Jacobian approximation.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

Return value The return value `flag` (of type `int`) is one of
`IDADENSE_SUCCESS` The optional output value has been successfuly set.
`IDADENSE_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDADENSE_LMEM_NULL` The IDADENSE linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if the default `IDADenseDQJac` difference quotient function is used.

`IDADenseGetLastFlag`

Call `flag = IDADenseGetLastFlag(ida_mem, &flag);`

Description The function `IDADenseGetLastFlag` returns the last return value from an IDADENSE routine.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`flag` (`int`) the value of the last return flag from an IDADENSE function.

Return value The return value `flag` (of type `int`) is one of

`IDADENSE_SUCCESS` The optional output value has been successfully set.
`IDADENSE_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDADENSE_LMEM_NULL` The IDADENSE linear solver has not been initialized.

Notes If the IDADENSE setup function failed (`IDASolve` returned `IDA_LSETUP_FAIL`), the value `flag` is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the dense Jacobian matrix.

`IDADenseGetReturnFlagName`

Call `name = IDADenseGetReturnFlagName(flag);`

Description The function `IDADenseGetReturnFlagName` returns the name of the CVDENSE constant corresponding to `flag`.

Arguments The only argument, of type `int` is a return flag from a CVDENSE function.

Return value The return value is a string containing the name of the corresponding constant.

5.5.8.5 Band linear solver

The following optional outputs are available from the IDABAND module: workspace requirements, number of calls to the Jacobian routine, number of calls to the residual routine for finite-difference Jacobian approximation, and last return value from a IDABAND function.

`IDABandGetWorkSpace`

Call `flag = IDABandGetWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDABandGetWorkSpace` returns the sizes of the IDABAND real and integer workspaces.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`lenrwKS` (`long int`) the number of real values in the IDABAND workspace.
`leniwLS` (`long int`) the number of integer values in the IDABAND workspace.

Return value The return value `flag` (of type `int`) is one of

`IDABAND_SUCCESS` The optional output value has been successfuly set.
`IDABAND_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDABAND_LMEM_NULL` The IDABAND linear solver has not been initialized.

Notes In terms of the problem size N and Jacobian half-bandwidths, the actual size of the real workspace is $N\,(2\,$`mupper`$+3\,$`mlower`$\,+2)$ `realtype` words. The actual size of the integer workspace is N integer words.

`IDABandGetNumJacEvals`

Call `flag = IDABandGetNumJacEvals(ida_mem, &njevals);`

Description The function `IDABandGetNumJacEvals` returns the cumulative number of calls to the banded Jacobian approximation function.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`njevals` (`long int`) the cumulative number of calls to the Jacobian function.

Return value The return value `flag` (of type `int`) is one of

`IDABAND_SUCCESS` The optional output value has been successfuly set.
`IDABAND_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDABAND_LMEM_NULL` The IDABAND linear solver has not been initialized.

`IDABandGetNumResEvals`

Call `flag = IDABandGetNumResEvals(ida_mem, &nrevalsLS);`

Description The function `IDABandGetNumResEvals` returns the cumulative number of calls to the user residual function due to the finite difference banded Jacobian approximation.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfuly set.
`IDABAND_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDABAND_LMEM_NULL`	The IDABAND linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if the default `IDABandDQJac` difference quotient function is used.

`IDABandGetLastFlag`

Call `flag = IDABandGetLastFlag(ida_mem, &flag);`

Description The function `IDABandGetLastFlag` returns the last return value from an IDABAND routine.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`flag` (`int`) the value of the last return flag from an IDABAND function.

Return value The return value `flag` (of type `int`) is one of

`IDABAND_SUCCESS`	The optional output value has been successfully set.
`IDABAND_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDABAND_LMEM_NULL`	The IDABAND linear solver has not been initialized.

Notes If the IDABAND setup function failed (`IDASolve` returned `IDA_LSETUP_FAIL`), the value `flag` is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the banded Jacobian matrix.

`IDABandGetReturnFlagName`

Call `name = IDABandGetReturnFlagName(flag);`

Description The function `IDABandGetReturnFlagName` returns the name of the CVBAND constant corresponding to `flag`.

Arguments The only argument, of type `int` is a return flag from a CVBAND function.

Return value The return value is a string containing the name of the corresponding constant.

5.5.8.6 SPILS linear solvers

The following optional outputs are available from the IDASPILS modules: workspace requirements, number of linear iterations, number of linear convergence failures, number of calls to the preconditioner setup and solve routines, number of calls to the Jacobian-vector product routine, number of calls to the residual routine for finite-difference Jacobian-vector product approximation, and last return value from a linear solver function.

`IDASpilsGetWorkSpace`

Call `flag = IDASpilsGetWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDASpilsGetWorkSpace` returns the global sizes of the IDASPGMR real and integer workspaces.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`lenrwLS` (`long int`) global number of real values in the IDASPILS workspace.
`leniwLS` (`long int`) global number of integer values in the IDASPILS workspace.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes In terms of the problem size N and maximum subspace size `maxl`, the actual size of the real workspace is roughly:
$N *$ (`maxl` $+5)+$ `maxl` $*($ `maxl` $+4) + 1$ `realtype` words for IDASPGMR,
$10 * N$ `realtype` words for IDASPBCG,
and $13 * N$ `realtype` words for IDASPTFQMR.

In a parallel setting, the above values are global — summed over all processors.

`IDASpilsGetNumLinIters`

Call `flag = IDASpilsGetNumLinIters(ida_mem, &nliters);`

Description The function `IDASpilsGetNumLinIters` returns the cumulative number of linear iterations.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nliters` (`long int`) the current number of linear iterations.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumConvFails`

Call `flag = IDASpilsGetNumConvFails(ida_mem, &nlcfails);`

Description The function `IDASpilsGetNumConvFails` returns the cumulative number of linear convergence failures.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nlcfails` (`long int`) the current number of linear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumPrecEvals`

Call `flag = IDASpilsGetNumPrecEvals(ida_mem, &npevals);`

Description The function `IDASpilsGetNumPrecEvals` returns the cumulative number of preconditioner evaluations, i.e., the number of calls made to `psetup`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`npevals` (`long int`) the cumulative number of calls to `psetup`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumPrecSolves`

Call `flag = IDASpilsGetNumPrecSolves(ida_mem, &npsolves);`

Description The function `IDASpilsGetNumPrecSolves` returns the cumulative number of calls made to the preconditioner solve function, `psolve`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`npsolves` (`long int`) the cumulative number of calls to `psolve`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumJtimesEvals`

Call `flag = IDASpilsGetNumJtimesEvals(ida_mem, &njvevals);`

Description The function `IDASpilsGetNumJtimesEvals` returns the cumulative number of calls made to the Jacobian-vector function, `jtimes`.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`njvevals` (`long int`) the cumulative number of calls to `jtimes`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumResEvals`

Call `flag = IDASpilsGetNumResEvals(ida_mem, &nrevalsLS);`

Description The function `IDASpilsGetNumResEvals` returns the cumulative number of calls to the user residual function for finite difference Jacobian-vector product approximation.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfuly set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if the default `IDASpilsDQJtimes` difference quotient function is used.

`IDASpilsGetLastFlag`

Call `flag = IDASpilsGetLastFlag(ida_mem, &flag);`

Description The function `IDASpilsGetLastFlag` returns the last return value from an IDASPILS routine.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`flag` (`int`) the value of the last return flag from an IDASPILS function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes If the IDASPILS setup function failed (`IDASolve` returned `IDA_LSETUP_FAIL`), `flag` will be `SPGMR_PSET_FAIL_UNREC`, `SPBCG_PSET_FAIL_UNREC`, or `SPTFQMR_PSET_FAIL_UNREC`.

If the IDASPGMR solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `flag` contains the error return flag from `SpgmrSolve` and will be one of: `SPGMR_MEM_NULL`, indicating that the SPGMR memory is `NULL`; `SPGMR_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J * v$ function; `SPGMR_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably; `SPGMR_GS_FAIL`, indicating a failure in the Gram-Schmidt procedure; or `SPGMR_QRSOL_FAIL`, indicating that the matrix R was found to be singular during the QR solve phase.

If the IDASPBCG solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `flag` contains the error return flag from `SpbcgSolve` and will be one of: `SPBCG_MEM_NULL`, indicating that the SPBCG memory is `NULL`; `SPBCG_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J * v$ function; or `SPBCG_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably.

If the IDASPTFQMR solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `flag` contains the error flag from `SptfqmrSolve` and will be one of: `SPTFQMR_MEM_NULL`, indicating that the SPTFQMR memory is `NULL`; `SPTFQMR_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J*v$ function; or `SPTFQMR_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably.

`IDASpilsGetReturnFlagName`

Call `name = IDASpilsGetReturnFlagName(flag);`

Description The function `IDASpilsGetReturnFlagName` returns the name of the CVSPILS constant corresponding to `flag`.

Arguments The only argument, of type `int` is a return flag from a CVSPILS function.

Return value The return value is a string containing the name of the corresponding constant.

5.5.9 IDA reinitialization function

The function `IDAReInit` reinitializes the main IDA solver for the solution of a problem, where a prior call to `IDAMalloc` has been made. The new problem must have the same size as the previous one. `IDAReInit` performs the same input checking and initializations that `IDAMalloc` does, but does no memory allocation, assuming that the existing internal memory is sufficient for the new problem.

The use of `IDAReInit` requires that the maximum method order, `maxord`, is no larger for the new problem than for the problem specified in the last call to `IDAMalloc`. In addition, the same NVECTOR module set for the previous problem will be reused for the new problem.

If there are changes to the linear solver specifications, make the appropriate `Set` calls, as described in §5.5.3.

IDAReInit

Call `flag = IDAReInit(ida_mem, res, t0, y0, yp0, itol, reltol, abstol);`

Description The function `IDAReInit` provides required problem specifications and reinitializes IDA.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `res` (`IDAResFn`) is the C function which computes F. This function has the form `f(t, y, yp, r, res_data)` (for full details see §5.6).
- `t0` (`realtype`) is the initial value of t.
- `y0` (`N_Vector`) is the initial value of y.
- `yp0` (`N_Vector`) is the initial value of y'.
- `itol` (`int`) is one of `IDA_SS`, `IDA_SV`, or `IDA_WF`, where `IDA_SS` indicates scalar relative error tolerance and scalar absolute error tolerance, while `IDA_SV` indicates scalar relative error tolerance and vector absolute error tolerance. The latter choice is important when the absolute error tolerance needs to be different for each component of the DAE. If `itol=IDA_WF`, the arguments `reltol` and `abstol` are ignored and the user is expected to provide a function to evaluate the error weight vector W as an alternative to Eq. (3.6). See `IDASetEwtFn` in §5.5.6.1.
- `reltol` (`realtype`) is the relative error tolerance.
- `abstol` (`void *`) is a pointer to the absolute error tolerance. If `itol=IDA_SS`, `abstol` must be a pointer to a `realtype` variable. If `itol=IDA_SV`, `abstol` must be an `N_Vector` variable.

Return value The return flag `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAReInit` was successful.
- `IDA_MEM_NULL` The IDA memory block was not initialized through a previous call to `IDACreate`.
- `IDA_NO_MALLOC` Memory space for the IDA memory block was not allocated through a previous call to `IDAMalloc`.
- `IDA_ILL_INPUT` An input argument to `IDAReInit` has an illegal value.

Notes If an error occurred, `IDAReInit` also sends an error message to the error handler function.

It is the user's responsibility to provide compatible `itol` and `abstol` arguments.

5.6 User-supplied functions

The user-supplied functions consist of one function defining the DAE residual, (optionally) a function that provides the error weight vector, (optionally) a function that provides Jacobian-related information for the linear solver (if Newton iteration is chosen), and (optionally) one or two functions that define the preconditioner for use in any of the Krylov iteration algorithms.

5.6.1 Residual function

The user must provide a function of type `IDAResFn` defined as follows:

IDAResFn

Definition
```
typedef int (*IDAResFn)(realtype tt, N_Vector yy, N_Vector yp,
                        N_Vector rr, void *res_data);
```

Purpose This function computes the problem residual for given values of the independent variable t, state vector y, and derivative y'.

Arguments `tt` is the current value of the independent variable.

yy is the current value of the dependent variable vector, $y(t)$.

yp is the current value of $y'(t)$.

rr is the output residual vector $F(t, y, y')$.

res_data is a pointer to user data — the same as the res_data parameter passed to IDASetRdata.

Return value An IDAResFn function type should return a value of 0 if successful, a positive value if a recoverable error occured (e.g. yy has an illegal value), or a negative value if a nonrecoverable error occured.

In the latter case, the integrator halts. If a recoverable error occured, the integrator will attempt to correct and retry.

Notes Allocation of memory for yp is handled within IDA.

5.6.2 Error message handler function

As an alternative to the default behavior of directing error and warning messages to the file pointed to by errfp (see IDASetErrFile), the user may provide a function of type IDAErrHandlerFn to process any such messages. The function type IDAErrHandlerFn is defined as follows:

IDAErrHandlerFn

Definition
```
typedef void (*IDAErrHandlerFn)(int error_code,
                                const char *module, const char *function,
                                char *msg, void *eh_data);
```

Purpose This function processes error and warning messages from IDA and its sub-modules.

Arguments error_code is the error code.

module is the name of the IDA module reporting the error.

function is the name of the function in which the error occurred.

msg is the error message.

eh_data is a pointer to user data, the same as the eh_data parameter passed to IDASetErrHandlerFn.

Return value A IDAErrHandlerFn function has no return value.

Notes error_code is negative for errors and positive (IDA_WARNING) for warnings. If a function returning a pointer to memory (e.g. IDABBDPrecAlloc) encounters an error, it sets error_code to 0 before returning NULL.

5.6.3 Error weight function

As an alternative to providing the relative and absolute tolerances, the user may provide a function of type IDAEwtFn to compute a vector ewt containing the multiplicative weights W_i used in the WRMS norm $\| v\|_{\text{WRMS}} = \sqrt{(1/N)\sum_1^N (W_i \cdot v_i)^2}$. These weights will used in place of those defined by Eq. (3.6). The function type IDAEwtFn is defined as follows:

IDAEwtFn

Definition
```
typedef int (*IDAEwtFn)(N_Vector y, N_Vector ewt, void *e_data);
```

Purpose This function computes the WRMS error weights for the vector y.

Arguments y is the value of the vector for which the WRMS norm must be computed.

ewt is the output vector containing the error weights.

e_data is a pointer to user data — the same as the e_data parameter passed to IDASetEwtFn.

Return value An `IDAEwtFn` function type must return 0 if it successfuly set the error weights and −1 otherwise. In case of failure, a message is printed and the integration stops.

Notes Allocation of memory for `ewt` is handled within IDA.

The error weight vector must have all components positive. It is the user's responsiblity to perform this test and return −1 if it is not satisfied.

5.6.4 Jacobian information (direct method with dense Jacobian)

If the direct linear solver with dense treatment of the Jacobian is used (i.e. `IDADense` is called in Step 7 of §5.4), the user may provide a function of type `IDADenseJacFn` defined by

`IDADenseJacFn`

Definition
```
typedef int (*IDADenseJacFn)(long int Neq, realtype tt,
                             N_Vector yy, N_Vector yp, N_Vector rr,
                             realtype c_j, void *jac_data, DenseMat Jac,
                             N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the dense Jacobian J of the DAE system (or an approximation to it), defined by Eq. (3.5).

Arguments
- `Neq` is the problem size (number of equations).
- `tt` is the current value of the independent variable t.
- `yy` is the current value of the dependent variable vector, $y(t)$.
- `yp` is the current value of $y'(t)$.
- `rr` is the current value of the residual vector $F(t, y, y')$.
- `c_j` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (3.5)).
- `jac_data` is a pointer to user data — the same as the `jac_data` parameter passed to `IDADenseSetJacFn`.
- `Jac` is the output Jacobian matrix.
- `tmp1`, `tmp2`, `tmp3` are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADenseJacFn` as temporary storage or work space.

Return value An `IDADenseJacFn` function type should return 0 if successful, a positive value if a recoverable error occured, or a negative value if a nonrecoverable error occured.

In the case of a recoverable eror return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (3.5).

Notes A user-supplied dense Jacobian function must load the `Neq` × `Neq` dense matrix `Jac` with an approximation to the Jacobian matrix J at the point (`tt`, `yy`, `yp`). Only nonzero elements need to be loaded into `Jac` because `Jac` is set to the zero matrix before the call to the Jacobian function. The type of `Jac` is `DenseMat` (described below and in §9.1).

The accessor macros `DENSE_ELEM` and `DENSE_COL` allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the `DenseMat` type. `DENSE_ELEM(Jac, i, j)` references the (`i`, `j`)-th element of the dense matrix `Jac` (`i`, `j`= 0 . . . `Neq`−1). This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to `Neq`, the Jacobian element $J_{m,n}$ can be loaded with the statement `DENSE_ELEM(Jac, m-1, n-1)` = $J_{m,n}$. Alternatively, `DENSE_COL(Jac, j)` returns a pointer to the storage for the `j`th column of `Jac` (`j`= 0 . . . `Neq`−1), and the elements of the `j`-th column are then accessed via ordinary array indexing. Thus $J_{m,n}$ can be loaded with the statements `col_n = DENSE_COL(Jac, n-1); col_n[m-1]` = $J_{m,n}$. For

large problems, it is more efficient to use DENSE_COL than to use DENSE_ELEM. Note that both of these macros number rows and columns starting from 0, not 1.

The DenseMat type and the accessor macros DENSE_ELEM and DENSE_COL are documented in §9.1.

If the user's IDADenseJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, use the IDAGet* functions described in §5.5.8.1. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

5.6.5 Jacobian information (direct method with banded Jacobian)

If the direct linear solver with banded treatment of the Jacobian is used (i.e. IDABand is called in Step 7 of §5.4), the user may provide a function of type IDABandJacFn defined as follows:

IDABandJacFn

Definition
```
typedef int (*IDABandJacFn)(long int Neq, long int mupper,
                            long int mlower, realtype tt,
                            N_Vector yy, N_Vector yp, N_Vector rr,
                            realtype c_j, void *jac_data, BandMat Jac,
                            N_Vector tmp1, N_Vector tmp2,N_Vector tmp3);
```

Purpose This function computes the banded Jacobian J of the DAE system (or a banded approximation to it), defined by Eq. (3.5).

Arguments

Neq	is the problem size.
mlower	
mupper	are the lower and upper half bandwidth of the Jacobian.
tt	is the current value of the independent variable.
yy	is the current value of the dependent variable vector, $y(t)$.
yp	is the current value of $y'(t)$.
rr	is the current value of the residual vector $F(t, y, y')$.
c_j	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (3.5)).
jac_data	is a pointer to user data — the same as the jac_data parameter passed to IDABandSetJacFn.
Jac	is the output Jacobian matrix.
tmp1	
tmp2	
tmp3	are pointers to memory allocated for variables of type N_Vector which can be used by IDABandJacFn as temporary storage or work space.

Return value A IDABandJacFn function type should return 0 if successful, a positive value if a recoverable error occured, or a negative value if a nonrecoverable error occured.

In the case of a recoverable eror return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (3.5).

Notes A user-supplied band Jacobian function must load the band matrix Jac of type BandMat with the elements of the Jacobian $J(t, y, y')$ at the point (tt, yy, yp). Only nonzero elements need to be loaded into Jac because Jac is preset to zero before the call to the Jacobian function.

The accessor macros BAND_ELEM, BAND_COL, and BAND_COL_ELEM allow the user to read and write band matrix elements without making specific references to the underlying representation of the BandMat type. BAND_ELEM(Jac, i, j) references the (i, j)th

element of the band matrix Jac, counting from 0. This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to Neq with (m, n) within the band defined by mupper and mlower, the Jacobian element $J_{m,n}$ can be loaded with the statement BAND_ELEM(Jac, m-1, n-1) = $J_{m,n}$. The elements within the band are those with -mupper $\leq$ m-n $\leq$ mlower. Alternatively, BAND_COL(Jac, j) returns a pointer to the diagonal element of the jth column of Jac, and if we assign this address to realtype *col_j, then the ith element of the jth column is given by BAND_COL_ELEM(col_j, i, j), counting from 0. Thus for (m, n) within the band, $J_{m,n}$ can be loaded by setting col_n = BAND_COL(Jac, n-1); BAND_COL_ELEM(col_n, m-1, n-1) = $J_{m,n}$. The elements of the jth column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type BandMat. The array col_n can be indexed from $-$mupper to mlower. For large problems, it is more efficient to use the combination of BAND_COL and BAND_COL_ELEM than to use the BAND_ELEM. As in the dense case, these macros all number rows and columns starting from 0, not 1.

The BandMat type and the accessor macros BAND_ELEM, BAND_COL, and BAND_COL_ELEM are documented in §9.2.

If the user's IDABandJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, use the IDAGet* functions described in §5.5.8.1. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

5.6.6 Jacobian information (matrix-vector product)

If one of the Krylov iterative linear solvers SPGMR, SPBCG, or SPTFQMR is selected (IDASp* is called in step 7 of §5.4), the user may provide a function of type IDASpilsJacTimesVecFn in the following form:

IDASpilsJacTimesVecFn

Definition
```
typedef int (*IDASpilsJacTimesVecFn)(realtype tt, N_Vector yy,
                                     N_Vector yp, N_Vector rr,
                                     N_Vector v, N_Vector Jv,
                                     realtype c_j, void *jac_data,
                                     N_Vector tmp1, N_Vector tmp2);
```

Purpose This function computes the product Jv of the DAE system Jacobian J (or an approximation to it) and a given vector v, where J is defined by Eq. (3.5).

Arguments

tt	is the current value of the independent variable.
yy	is the current value of the dependent variable vector, $y(t)$.
yp	is the current value of $y'(t)$.
rr	is the current value of the residual vector $F(t, y, y')$.
v	is the vector by which the Jacobian must be multiplied to the right.
Jv	is the output vector computed.
c_j	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (3.5)).
jac_data	is a pointer to user data — the same as the jac_data parameter passed to IDASp*SetJacTimesVecFn.
tmp1	
tmp2	are pointers to memory allocated for variables of type N_Vector which can be used by IDASpilsJacTimesVecFn as temporary storage or work space.

Return value The value to be returned by the Jacobian-times-vector function should be 0 if successful. A nonzero value indicates that a nonrecoverable error occurred.

If the user's `IDASpilsJacTimesVecFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, use the `IDAGet*` functions described in §5.5.8.1. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

5.6.7 Preconditioning (linear system solution)

If preconditioning is used, then the user must provide a C function to solve the linear system $Pz = r$ where P is a left preconditioner matrix which approximates (at least crudely) the Jacobian matrix $J = \partial F/\partial y + c_j \partial F/\partial y'$. This function must be of type `IDASpilsPrecSolveFn`, defined as follows:

`IDASpilsPrecSolveFn`

Definition
```
typedef int (*IDASpilsPrecSolveFn)(realtype tt, N_Vector yy,
                                   N_Vector yp, N_Vector rr,
                                   N_Vector rvec, N_Vector zvec,
                                   realtype c_j, realtype delta,
                                   void *p_data, N_Vector tmp);
```

Purpose This function solves the preconditioning system $Pz = r$.

Arguments
- `tt` is the current value of the independent variable.
- `yy` is the current value of the dependent variable vector, $y(t)$.
- `yp` is the current value of $y'(t)$.
- `rr` is the current value of the residual vector $F(t, y, y')$.
- `rvec` is the right-hand side vector r of the linear system to be solved.
- `zvec` is the output vector computed.
- `c_j` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (3.5)).
- `delta` is an input tolerance to be used if an iterative method is employed in the solution. In that case, the residual vector $Res = r - Pz$ of the system should be made less than `delta` in weighted l_2 norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} <$ `delta`. To obtain the `N_Vector ewt`, call `IDAGetErrWeights` (see §5.5.8.1).
- `p_data` is a pointer to user data — the same as the `p_data` parameter passed to the function `IDASp*SetPreconditioner`.
- `tmp` is a pointer to memory allocated for a variable of type `N_Vector` which can be used for work space.

Return value The value to be returned by the preconditioner solve function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), negative for an unrecoverable error (in which case the integration is halted).

5.6.8 Preconditioning (Jacobian data)

If the user's preconditioner requires that any Jacobian-related data be evaluated or preprocessed, then this needs to be done in a user-supplied C function of type `IDASpilsPrecSetupFn`, defined as follows:

`IDASpilsPrecSetupFn`

Definition
```
typedef int (*IDASpilsPrecSetupFn)(realtype tt, N_Vector yy,
                                   N_Vector yp, N_Vector rr,
                                   realtype c_j, void *p_data,
                                   N_Vector tmp1, N_Vector tmp2,
                                   N_Vector tmp3);
```

Purpose This function evaluates and/or preprocesses Jacobian-related data needed by the preconditioner.

Arguments The arguments of an `IDASpilsPrecSetupFn` are as follows:

- `tt` is the current value of the independent variable.
- `yy` is the current value of the dependent variable vector, $y(t)$.
- `yp` is the current value of $y'(t)$.
- `rr` is the current value of the residual vector $F(t, y, y')$.
- `c_j` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (3.5)).
- `p_data` is a pointer to user data — the same as the `p_data` parameter passed to the function `IDASp*SetPreconditioner`.
- `tmp1`
- `tmp2`
- `tmp3` are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDASpilsPrecSetupFn` as temporary storage or work space.

Return value The value to be returned by the preconditioner setup function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), negative for an unrecoverable error (in which case the integration is halted).

Notes The operations performed by this function might include forming a crude approximate Jacobian, and performing an LU factorization on the resulting approximation.

Each call to the preconditioner setup function is preceded by a call to the `IDAResFn` user function with the same (`tt`, `yy`, `yp`) arguments. Thus the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual.

This function is not called in advance of every call to the preconditioner solve function, but rather is called only as often as needed to achieve convergence in the Newton iteration.

If the user's `IDASpilsPrecSetupFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, use the `IDAGet*` functions described in §5.5.8.1. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

5.7 Rootfinding

While integrating the IVP, IDA has the capability of finding the roots of a set of user-defined functions. This section describes the user-callable functions used to initialize and define the rootfinding problem and obtain solution information, and it also describes the required additional user-supplied function.

5.7.1 User-callable functions for rootfinding

`IDARootInit`

Call `flag = IDARootInit(ida_mem, nrtfn, g, g_data);`

Description The function `IDARootInit` specifies that the roots of a set of functions $g_i(t, y, y')$ are to be found while the IVP is being solved.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block returned by `IDACreate`.
- `nrtfn` (`int`) is the number of root functions g_i.
- `g` (`IDARootFn`) is the C function which defines the `nrtfn` functions $g_i(t, y, y')$ whose roots are sought. See §5.7.2 for details.
- `g_data` (`void *`) pointer to the user data for use by the user's root function g.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The call to `IDARootInit` was successful.
- `IDA_MEM_NULL` The `ida_mem` argument was `NULL`.
- `IDA_MEM_FAIL` A memory allocation failed.
- `IDA_ILL_INPUT` The function `g` is `NULL`, but `nrtfn`> 0.

Notes If a new IVP is to be solved with a call to `IDAReInit`, where the new IVP has no rootfinding problem but the prior one did, then call `IDARootInit` with `nrtfn`$= 0$.

There are two optional output functions associated with rootfinding.

`IDAGetRootInfo`

Call `flag = IDAGetRootInfo(ida_mem, rootsfound);`

Description The function `IDAGetRootInfo` returns an array showing which functions were found to have a root.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `rootsfound` (`int *`) array of length `nrtfn` with the indices of the user functions g_i found to have a root. For $i = 0, \ldots,$`nrtfn` -1, `rootsfound`$[i] = 1$ if g_i has a root, and $= 0$ if not.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The optional output values have been successfully set.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The user must allocate memory for the vector `rootsfound`.

`IDAGetNumGEvals`

Call `flag = IDAGetNumGEvals(ida_mem, &ngevals);`

Description The function `IDAGetNumGEvals` returns the cumulative number of calls to the user root function g.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `ngevals` (`long int`) number of calls to the user's function `g` so far.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The optional output value has been successfully set.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

5.7.2 User-supplied function for rootfinding

If a rootfinding problem is to be solved during the integration of the ODE system, the user must supply a C function of type `IDARootFn`, defined as follows:

IDARootFn

Definition
```
typedef int (*IDARootFn)(realtype t, N_Vector y, N_Vector yp,
                         realtype *gout, void *g_data);
```

Purpose This function computes a vector-valued function $g(t, y, y')$ such that the roots of the nrtfn components $g_i(t, y, y')$ are to be found during the integration.

Arguments
- t is the current value of the independent variable.
- y is the current value of the dependent variable vector, $y(t)$.
- yp is the current value of $y'(t)$, the $t-$derivative of y.
- gout is the output array, of length nrtfn, with components $g_i(t, y, y')$.
- g_data is a pointer to user data — the same as the g_data parameter passed to IDARootInit.

Return value An IDARootFn should return 0 if successful or a non-zero value if an error occured (in which case the integration is halted and IDASolve returns IDA_RTFUNC_FAIL).

Notes Allocation of memory for gout is handled within IDA.

5.8 A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel DAE solver such as IDA lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (3.4) that must be solved at each time step. The linear algebraic system is large, sparse, and structured. However, if a Krylov iterative method is to be effective in this setting, then a nontrivial preconditioner needs to be used. Otherwise, the rate of convergence of the Krylov iterative method is usually unacceptably slow. Unfortunately, an effective preconditioner tends to be problem-specific.

However, we have developed one type of preconditioner that treats a rather broad class of PDE-based problems. It has been successfully used for several realistic, large-scale problems [15] and is included in a software module within the IDA package. This module works with the parallel vector module NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix. The blocks need not have the same number of super- and sub-diagonals and these numbers may vary from block to block. This Band-Block-Diagonal Preconditioner module is called IDABBDPRE.

One way to envision these preconditioners is to think of the domain of the computational PDE problem as being subdivided into M non-overlapping sub-domains. Each of these sub-domains is then assigned to one of the M processors to be used to solve the DAE system. The basic idea is to isolate the preconditioning so that it is local to each processor, and also to use a (possibly cheaper) approximate residual function. This requires the definition of a new function $G(t, y, y')$ which approximates the function $F(t, y, y')$ in the definition of the DAE system (3.1). However, the user may set $G = F$. Corresponding to the domain decomposition, there is a decomposition of the solution vectors y and y' into M disjoint blocks y_m and y'_m, and a decomposition of G into blocks G_m. The block G_m depends on y_m and y'_m, and also on components of $y_{m'}$ and $y'_{m'}$ associated with neighboring sub-domains (so-called ghost-cell data). Let $\bar{y}_m$ and $\bar{y'}_m$ denote y_m and y'_m (respectively) augmented with those other components on which G_m depends. Then we have

$$G(t, y, y') = [G_1(t, \bar{y}_1, \bar{y}'_1), G_2(t, \bar{y}_2, \bar{y}'_2), \ldots, G_M(t, \bar{y}_M, \bar{y}'_M)]^T \ , \tag{5.1}$$

and each of the blocks $G_m(t, \bar{y}_m, \bar{y}'_m)$ is uncoupled from the others.

The preconditioner associated with this decomposition has the form

$$P = diag[P_1, P_2, \ldots, P_M] \tag{5.2}$$

where

$$P_m \approx \partial G_m/\partial y_m + \alpha \partial G_m/\partial y'_m \tag{5.3}$$

This matrix is taken to be banded, with upper and lower half-bandwidths `mudq` and `mldq` defined as the number of non-zero diagonals above and below the main diagonal, respectively. The difference quotient approximation is computed using `mudq` + `mldq` +2 evaluations of G_m, but only a matrix of bandwidth `mukeep` + `mlkeep` +1 is retained.

Neither pair of parameters need be the true half-bandwidths of the Jacobians of the local block of G, if smaller values provide a more efficient preconditioner. Such an efficiency gain may occur if the couplings in the DAE system outside a certain bandwidth are considerably weaker than those within the band. Reducing `mukeep` and `mlkeep` while keeping `mudq` and `mldq` at their true values, discards the elements outside the narrower band. Reducing both pairs has the additional effect of lumping the outer Jacobian elements into the computed elements within the band, and requires more caution and experimentation.

The solution of the complete linear system

$$Px = b \tag{5.4}$$

reduces to solving each of the equations

$$P_m x_m = b_m \tag{5.5}$$

and this is done by banded LU factorization of P_m followed by a banded backsolve.

Similar block-diagonal preconditioners could be considered with different treatment of the blocks P_m. For example, incomplete LU factorization or an iterative method could be used instead of banded LU factorization.

The IDABBDPRE module calls two user-provided functions to construct P: a required function `Gres` (of type `IDABBDLocalFn`) which approximates the residual function $G(t, y, y') \approx F(t, y, y')$ and which is computed locally, and an optional function `Gcomm` (of type `IDABBDCommFn`) which performs all inter-process communication necessary to evaluate the approximate residual G. These are in addition to the user-supplied residual function `res`. Both functions take as input the same pointer `res_data` as passed by the user to `IDASetRdata` and passed to the user's function `res`, and neither function has a return value. The user is responsible for providing space (presumably within `res_data`) for components of `yy` and `yp` that are communicated by `Gcomm` from the other processors, and that are then used by `Gres`, which is not expected to do any communication.

`IDABBDLocalFn`

Definition
```
typedef int (*IDABBDLocalFn)(long int Nlocal, realtype tt,
                             N_Vector yy, N_Vector yp, N_Vector gval,
                             void *res_data);
```

Purpose This function computes $G(t, y, y')$. It loads the vector `gval` as a function of `tt`, `yy`, and `yp`.

Arguments
- `Nlocal` is the local vector length.
- `tt` is the value of the independent variable.
- `yy` is the dependent variable.
- `yp` is the derivative of the dependent variable.
- `gval` is the output vector.
- `res_data` is a pointer to user data — the same as the `res_data` parameter passed to `IDASetRdata`.

Return value An `IDABBDLocalFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes This function assumes that all inter-processor communication of data needed to calculate `gval` has already been done, and this data is accessible within `res_data`.

The case where G is mathematically identical to F is allowed.

IDABBDCommFn

Definition `typedef int (*IDABBDCommFn)(long int Nlocal, realtype tt, N_Vector yy, N_Vector yp, void *res_data);`

Purpose This function performs all inter-processor communications necessary for the execution of the `Gres` function above, using the input vectors `yy` and `yp`.

Arguments
- `Nlocal` is the local vector length.
- `tt` is the value of the independent variable.
- `yy` is the dependent variable.
- `yp` is the derivative of the dependent variable.
- `res_data` is a pointer to user data — the same as the `res_data` parameter passed to `IDASetRdata`.

Return value An `IDABBDCommFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes The `Gcomm` function is expected to save communicated data in space defined within the structure `res_data`.

Each call to the `Gcomm` function is preceded by a call to the residual function `res` with the same (`tt`, `yy`, `yp`) arguments. Thus `Gcomm` can omit any communications done by `res` if relevant to the evaluation of `Gres`. If all necessary comunication was done in `res`, then `Gcomm` = `NULL` can be passed in the call to `IDABBDPrecAlloc` (see below).

Besides the header files required for the integration of the DAE problem (see §5.3), to use the IDABBDPRE module, the main program must include the header file `ida_bbdpre.h` which declares the needed function prototypes.

The following is a summary of the usage of this module and describes the sequence of calls in the user main program. Steps that are unchanged from the user main program presented in §5.4 are grayed-out.

1. **Initialize MPI**
2. **Set problem dimensions**
3. **Set vector of initial values**
4. **Create IDA object**
5. **Allocate internal memory**
6. **Set optional inputs**
7. **Initialize the IDABBDPRE preconditioner module**

   Specify the upper and lower bandwidths `mudq`, `mldq` and `mukeep`, `mlkeep` and call

   ```
   bbd_data = IDABBDPrecAlloc(ida_mem, Nlocal, mudq, mldq,
                              mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);
   ```

   to allocate memory for and initialize a data structure `bbd_data`, of type `void *`, to be passed to any of the Krylov linear solvers. The last two arguments of `IDABBDPrecAlloc` are the two user-supplied functions described above.

8. **Attach iterative linear solver, one of:**

   (a) `flag = IDABBDSpgmr(ida_mem, maxl, bbd_data);`

   (b) `flag = IDABBDSpbcg(ida_mem, maxl, bbd_data);`

   (c) `flag = IDABBDSptfqmr(ida_mem, maxl, bbd_data);`

The function IDABBDSp* is a wrapper around the specification function IDASp* and performs the following actions:

- Attaches the IDASPGMR, IDASPBCG, or IDASPTFQMR linear solver to the main IDA solver memory;
- Sets the preconditioner data structure for IDABBDPRE;
- Sets the preconditioner setup function for IDABBDPRE;
- Sets the preconditioner solve function for IDABBDPRE;

9. **Set linear solver optional inputs**

   Note that the user should not overwrite the preconditioner data, setup function, or solve function through calls to IDASPGMR, IDASPBCG, or IDASPTFQMR optional input functions.

10. **Correct initial values**

11. **Specify rootfinding problem**

12. **Advance solution in time**

13. **Get optional outputs**

    Additional optional outputs associated with IDABBDPRE are available by way of two routines described below – IDABBDPreconGetWorkSpace and IDABBDPreconGetNumGfnEvals.

14. **Deallocate memory for solution vector**

15. **Free the IDABBDPRE data structure**

```
IDABBDPrecFree(&bbd_data);
```

16. **Free solver memory**

17. **Finalize MPI**

The user-callable functions that initialize, attach, and deallocate the IDABBDPRE preconditioner module (steps 7, 8, and 15 above) are described next.

IDABBDPrecAlloc

Call
```
bbd_data = IDABBDPrecAlloc(ida_mem, Nlocal, mudq, mldq,
                           mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);
```

Description The function IDABBDPrecAlloc initializes and allocates memory for the IDABBDPRE preconditioner.

Arguments

ida_mem	(void *) pointer to the IDA memory block.
Nlocal	(long int) local vector dimension.
mudq	(long int) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
mldq	(long int) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
mukeep	(long int) upper half-bandwidth of the retained banded approximate Jacobian block.
mlkeep	(long int) lower half-bandwidth of the retained banded approximate Jacobian block.
dq_rel_yy	(realtype) the relative increment in components of y used in the difference quotient approximations. The default is dq_rel_yy= $\sqrt{\text{unit roundoff}}$, which can be specified by passing dq_rel_yy= 0.0.

`Gres` (`IDABBDLocalFn`) the C function which computes the local residual approximation $G(t, y, y')$.

`Gcomm` (`IDABBDCommFn`) the optional C function which performs all inter-process communication required for the computation of $G(t, y, y')$.

Return value If successful, `IDABBDPrecAlloc` returns a pointer to the newly created IDABBDPRE memory block (of type `void *`). If an error occurred, `IDABBDPrecAlloc` returns `NULL`.

Notes If one of the half-bandwidths `mudq` or `mldq` to be used in the difference-quotient calculation of the approximate Jacobian is negative or exceeds the value `Nlocal`-1, it is replaced by 0 or `Nlocal`-1 accordingly.

The half-bandwidths `mudq` and `mldq` need not be the true half-bandwidths of the Jacobian of the local block of G, when smaller values may provide a greater efficiency.

Also, the half-bandwidths `mukeep` and `mlkeep` of the retained banded approximate Jacobian block may be even smaller, to reduce storage and computation costs further.

For all four half-bandwidths, the values need not be the same on every processor.

`IDABBDSpgmr`

Call `flag = IDABBDSpgmr(ida_mem, maxl, bbd_data);`

Description The function `IDABBDSpgmr` links the IDABBDPRE data to the IDASPGMR linear solver and attaches the latter to the IDA memory block.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPGMR_MAXL`$= 5$.

`bbd_data` (`void *`) pointer to the IDABBDPRE data structure.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The IDASPGMR initialization was successful.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_MEM_FAIL`	A memory allocation request failed.
`IDABBDPRE_PDATA_NULL`	The IDABBDPRE preconditioner has not been initialized.

`IDABBDSpbcg`

Call `flag = IDABBDSpbcg(ida_mem, maxl, bbd_data);`

Description The function `IDABBDSpbcg` links the IDABBDPRE data to the IDASPBCG linear solver and attaches the latter to the IDA memory block.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPBCG_MAXL`$= 5$.

`bbd_data` (`void *`) pointer to the IDABBDPRE data structure.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The IDASPBCG initialization was successful.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_MEM_FAIL`	A memory allocation request failed.
`IDABBDPRE_PDATA_NULL`	The IDABBDPRE preconditioner has not been initialized.

`IDABBDSptfqmr`

Call `flag = IDABBDSptfqmr(ida_mem, maxl, bbd_data);`

Description The function `IDABBDSptfqmr` links the IDABBDPRE data to the IDASPTFQMR linear solver and attaches the latter to the IDA memory block.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPTFQMR_MAXL`= 5.
- `bbd_data` (`void *`) pointer to the IDABBDPRE data structure.

Return value The return value `flag` (of type `int`) is one of
- `IDASPILS_SUCCESS` The IDASPTFQMR initialization was successful.
- `IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDASPILS_MEM_FAIL` A memory allocation request failed.
- `IDABBDPRE_PDATA_NULL` The IDABBDPRE preconditioner has not been initialized.

`IDABBDPrecFree`

Call `IDABBDPrecFree(&bbd_data);`

Description The function `IDABBDPrecFree` frees the pointer allocated by `IDABBDPrecAlloc`.

Arguments The only argument of `IDABBDPrecFree` is the pointer to the IDABBDPRE data structure (of type `void *`).

Return value The function `IDABBDPrecFree` has no return value.

The IDABBDPRE module also provides a reinitialization function to allow for a sequence of problems of the same size with IDASPGMR/IDABBDPRE, IDASPBCG/IDABBDPRE, or IDASPTFQMR/IDABBDPRE, provided there is no change in `local_N`, `mukeep`, or `mlkeep`. After solving one problem, and after calling `IDAReInit` to re-initialize IDA for a subsequent problem, a call to `IDABBDPrecReInit` can be made to change any of the following: the half-bandwidths `mudq` and `mldq` used in the difference-quotient Jacobian approximations, the relative increment `dq_rel_yy`, or one of the user-supplied functions `Gres` and `Gcomm`.

`IDABBDPrecReInit`

Call `flag = IDABBDPrecReInit(bbd_data, mudq, mldq, dq_rel_yy, Gres, Gcomm);`

Description The function `IDABBDPrecReInit` reinitializes the IDABBDPRE preconditioner.

Arguments
- `bbd_data` (`void *`) pointer to the IDABBDPRE data structure.
- `mudq` (`long int`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mldq` (`long int`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `dq_rel_yy` (`realtype`) the relative increment in components of `y` used in the difference quotient approximations. The default is `dq_rel_yy` = $\sqrt{\text{unit roundoff}}$, which can be specified by passing `dq_rel_yy` = 0.0.
- `Gres` (`IDABBDLocalFn`) the C function which computes the local residual approximation $G(t, y, y')$.
- `Gcomm` (`IDABBDCommFn`) the optional C function which performs all inter-process communication required for the computation of $G(t, y, y')$.

Return value The return value of `IDABBDPrecReInit` is `IDABBDPRE_SUCCESS` indicating success, or `IDABBDPRE_PDATA_NULL` if `bbd_data` is `NULL`.

Notes If one of the half-bandwidths `mudq` or `mldq` is negative or exceeds the value `Nlocal`-1, it is replaced by 0 or `Nlocal`-1, accordingly.

The following two optional output functions are available for use with the IDABBDPRE module:

`IDABBDPrecGetWorkSpace`

Call `flag = IDABBDPrecGetWorkSpace(bbd_data, &lenrwBBDP, &leniwBBDP);`

Description The function `IDABBDPrecGetWorkSpace` returns the local sizes of the IDABBDPRE real and integer workspaces.

Arguments
`bbd_data` (`void *`) pointer to the IDABBDPRE data structure.
`lenrwBBDP` (`long int`) local number of real values in the IDABBDPRE workspace.
`leniwBBDP` (`long int`) local number of integer values in the IDABBDPRE workspace.

Return value The return value `flag` (of type `int`) is one of

`IDABBDPRE_SUCCESS`	The optional output value has been successfuly set.
`IDABBDPRE_PDATA_NULL`	The IDABBDPRE preconditioner has not been initialized.

Notes In terms of the local vector dimension N_l, and `smu` $= \min(N_l - 1,$ `mukeep` $+$ `mlkeep`$)$, the actual size of the real workspace is N_l (2 `mlkeep` $+$ `mukeep` $+$ `smu` $+2$) `realtype` words. The actual size of the integer workspace is N_l integer words.

`IDABBDPrecGetNumGfnEvals`

Call `flag = IDABBDPrecGetNumGfnEvals(bbd_data, &ngevalsBBDP);`

Description The function `IDABBDPrecGetNumGfnEvals` returns the cumulative number of calls to the user `Gres` function due to the finite difference approximation of the Jacobian blocks used within IDABBDPRE's preconditioner setup function.

Arguments
`bbd_data` (`void *`) pointer to the IDABBDPRE data structure.
`ngevalsBBDP` (`long int`) the cumulative number of calls to the user `Gres` function.

Return value The return value `flag` (of type `int`) is one of

`IDABBDPRE_SUCCESS`	The optional output value has been successfuly set.
`IDABBDPRE_PDATA_NULL`	The IDABBDPRE preconditioner has not been initialized.

`IDABandPrecGetReturnFlagName`

Call `name = IDABandPrecGetReturnFlagName(flag);`

Description The function `IDABandPrecGetReturnFlagName` returns the name of the CVBANDPRE constant corresponding to `flag`.

Arguments The only argument, of type `int` is a return flag from a CVBANDPRE function.

Return value The return value is a string containing the name of the corresponding constant.

In addition to the `ngevalsBBDP` `Gres` evaluations, the costs associated with IDABBDPRE also include `nlinsetups` LU factorizations, `nlinsetups` calls to `Gcomm`, `npsolves` banded backsolve calls, and `nrevalsLS` residual function evaluations, where `nlinsetups` is an optional IDA output (see §5.5.8.1), and `npsolves` and `nrevalsLS` are linear solver optional outputs (see §5.5.8.3).

Chapter 6

FIDA, an Interface Module for FORTRAN Applications

The FIDA interface module is a package of C functions which support the use of the IDA solver, for the solution of DAE systems, in a mixed FORTRAN/C setting. While IDA is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in FORTRAN. This package provides the necessary interface to IDA for both the serial and the parallel NVECTOR implementations.

6.1 FIDA routines

The user-callable functions, with the corresponding IDA functions, are as follows:

- Interface to the NVECTOR modules
  - `FNVINITS` (defined by NVECTOR_SERIAL) interfaces to `N_VNewEmpty_Serial`.
  - `FNVINITP` (defined by NVECTOR_PARALLEL) interfaces to `N_VNewEmpty_Parallel`.
- Interface to the main IDA module
  - `FIDAMALLOC` interfaces to `IDACreate` and `IDAMalloc`.
  - `FIDAREINIT` interfaces to `IDAReInit`.
  - `FIDASETIIN`, `FIDASETVIN`, and `FIDASETRIN` interface to `IDASet*` functions.
  - `FIDATOLREINIT` interfaces to `IDASetTolerances`.
  - `FIDACALCIC` interfaces to `IDACalcIC`.
  - `FIDAEWTSET` interfaces to `IDAEwtSetFn`.
  - `FIDASOLVE` interfaces to `IDASolve`, `IDAGet*` functions, and to the optional output functions for the selected linear solver module.
  - `FIDAGETSOL` interfaces to `IDAGetSolution`.
  - `FIDAGETERRWEIGHTS` interfaces to `IDAGetErrWeights`.
  - `FIDAGETESTLOCALERR` interfaces to `IDAGetEstLocalErrors`.
  - `FIDAFREE` interfaces to `IDAFree`.
- Interface to the linear solver modules
  - `FIDADENSE` interfaces to `IDADense`.
  - `FIDADENSESETJAC` interfaces to `IDADenseSetJacFn`.

- FIDABAND interfaces to IDABand.
- FIDABANDSETJAC interfaces to IDABandSetJacFn.
- FIDASPGMR interfaces to IDASpgmr and SPGMR optional input functions.
- FIDASPGMRREINIT interfaces to SPGMR optional input functions.
- FIDASPBCG interfaces to IDASpbcg and SPBCG optional input functions.
- FIDASPBCGREINIT interfaces to SPBCG optional input functions.
- FIDASPTFQMR interfaces to IDASptfqmr and SPTFQMR optional input functions.
- FIDASPTFQMRREINIT interfaces to SPTFQMR optional input functions.
- FIDASPILSSETJAC interfaces to IDASpilsSetJacTimesVecFn.
- FIDASPILSSETPREC interfaces to IDASpilsSetPreconditioner.

The user-supplied functions, each listed with the corresponding interface function which calls it (and its type within IDA), are as follows:

FIDA routine (FORTRAN)	IDA function (C)	IDA function type
FIDARESFUN	FIDAresfn	IDAResFn
FIDAEWT	FIDAEwtSet	IDAEwtFn
FIDADJAC	FIDADenseJac	IDADenseJacFn
FIDABJAC	FIDABandJac	IDABandJacFn
FIDAPSOL	FIDAPSol	IDASpilsPrecSolveFn
FIDAPSET	FIDAPSet	IDASpilsPrecSetupFn
FIDAJTIMES	FIDAJtimes	IDASpilsJacTimesVecFn

In contrast to the case of direct use of IDA, and of most FORTRAN DAE solvers, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program.

6.1.1 Important note on portability

In this package, the names of the interface functions, and the names of the FORTRAN user routines called by them, appear as dummy names which are mapped to actual values by a series of definitions in the header files fida.h, fidaroot.h, and fidabbd.h. By default, those mapping definitions depend in turn on the C macros F77_FUNC and F77_FUNC_ defined in the header file sundials_config.h by configure. However, the set of flags
SUNDIALS_CASE_UPPER, SUNDIALS_CASE_LOWER,
SUNDIALS_UNDERSCORE_NONE, SUNDIALS_UNDERSCORE_ONE, and SUNDIALS_UNDERSCORE_TWO
can be explicitly defined in the header file sundials_config.h when configuring SUNDIALS via the --with-f77underscore and --with-f77case options to override the default behavior if necessary (see Chapter 2). Either way, the names into which the dummy names are mapped are in upper or lower case and have up to two underscores appended.

The user must also ensure that variables in the user FORTRAN code are declared in a manner consistent with their counterparts in IDA. All real variables must be declared as REAL, DOUBLE PRECISION, or perhaps as REAL*n, where n denotes the number of bytes, depending on whether IDA was built in single, double, or extended precision (see Chapter 2). Moreover, some of the FORTRAN integer variables must be declared as INTEGER*4 or INTEGER*8 according to the C type long int. These integer variables include: the array of integer optional outputs (IOUT), problem dimensions (NEQ, NLOCAL, NGLOBAL), Jacobian half-bandwidths (MU, ML, etc.), as well as the array of user integer data, IPAR. This is particularly important when using IDA and the FIDA package on 64-bit architectures.

6.2 Usage of the FIDA interface module

The usage of FIDA requires calls to five or more interface functions, depending on the method options selected, and one or more user-supplied routines which define the problem to be solved. These function

calls and user routines are summarized separately below. Some details are omitted, and the user is referred to the description of the corresponding IDA functions for information on the arguments of any given user-callable interface routine, or of a given user-supplied function called by an interface function. The usage of FIDA for rootfinding, and usage of FIDA with preconditioner modules, are each described in later sections.

Steps marked with [**S**] in the instructions below apply to the serial NVECTOR implementation (NVECTOR_SERIAL) only, while those marked with [**P**] apply to NVECTOR_PARALLEL.

1. **Residual function specification**

   The user must in all cases supply the following FORTRAN routine

   ```
   SUBROUTINE FIDARESFUN (T, Y, YP, R, IPAR, RPAR, IER)
   DIMENSION Y(*), YP(*), R(*), IPAR(*), RPAR(*)
   ```

   It must set the `R` array to $F(t, y, y')$, the residual function of the DAE system, as a function of `T` $= t$ and the arrays `Y` $= y$ and `YP` $= y'$. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`. It should return `IER` $= 0$ if it was successful, `IER` $= 1$ if it had a recoverable failure, or `IER` $=$ -1 if it had a non-recoverable failure.

2. NVECTOR **module initialization**

   [**S**] To initialize the serial NVECTOR module, the user must make the following call:

   ```
   CALL FNVINITS (KEY, NEQ, IER)
   ```

   where `KEY` is the solver id (`KEY`=1 for IDA), `NEQ` is the size of vectors, and `IER` is a return flag, which is set to 0 on success and -1 if a failure occurred.

   [**P**] To initialize the parallel vector module, the user must make the following call:

   ```
   CALL FNVINITP (COMM, KEY, NLOCAL, NGLOBAL, IER)
   ```

   in which the arguments are: `COMM` = MPI communicator, `KEY` = 1, `NLOCAL` = the local size of all vectors on this processor, and `NGLOBAL` = the system size (and the global size of vectors, equal to the sum of all values of `NLOCAL`). The return flag `IER` is set to 0 on a successful return and to -1 otherwise.

   If the header file `sundials_config.h` defines `SUNDIALS_MPI_COMM_F2C` to be 1 (meaning the MPI implementation used to build SUNDIALS includes the `MPI_Comm_f2c` function), then `COMM` can be any valid MPI communicator. Otherwise, `MPI_COMM_WORLD` will be used, so just pass an integer value as a placeholder.

3. **Problem specification**

   To set various problem and solution parameters and allocate internal memory, make the following call:

   `FIDAMALLOC`

   Call
   ```
   CALL FIDAMALLOC(T0, Y0, YP0, IATOL, RTOL, ATOL,
   &                IOUT, ROUT, IPAR, RPAR, IER)
   ```
   Description This function provides required problem and solution specifications, specifies optional inputs, allocates internal memory, and initializes IDA.

   Arguments
   - `T0` is the initial value of t.
   - `Y0` is an array of initial conditions for y.
   - `YP0` is an array of initial conditions for y'.

IATOL specifies the type for absolute tolerance ATOL: 1 for scalar or 2 for array. If IATOL= 3, the arguments RTOL and ATOL are ignored and the user is expected to subsequently call FIDAEWTSET and provide the function FIDAEWT.
RTOL is the relative tolerance (scalar).
ATOL is the absolute tolerance (scalar or array).
IOUT is an integer array of length at least 21 for integer optional outputs.
ROUT is a real array of length at least 6 for real optional outputs.
IPAR is an integer array of user data which will be passed unmodified to all user-provided routines.
RPAR is a real array of user data which will be passed unmodified to all user-provided routines.

Return value IER is a return completion flag. Values are 0 for successful return and -1 otherwise. See printed message for details in case of failure.

Notes The user intger data array IPAR must be declared as INTEGER*4 or INTEGER*8 according to the C type long int.

Modifications to the user data arrays IPAR and RPAR inside a user-provided routine will be propagated to all subsequent calls to such routines.

The optional outputs associated with the main IDA integrator are listed in Table 6.2.

As an alternative to providing tolerances in the call to FIDAMALLOC, the user may provide a routine to compute the error weights used in the WRMS norm evaluations. If supplied, it must have the following form:

```
SUBROUTINE FIDAEWT (Y, EWT, IPAR, RPAR, IER)
DIMENSION Y(*), EWT(*), IPAR(*), RPAR(*)
```

It must set the positive components of the error weight vector EWT for the calculation of the WRMS norm of Y. On return, set IER $= 0$ if FIDAEWT was successful, and nonzero otherwise. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the FIDAEWT routine is provided, then, following the call to FIDAMALLOC, the user must make the call:

```
CALL FIDAEWTSET (FLAG, IER)
```

with FLAG $\neq 0$ to specify use of the user-supplied error weight routine. The argument IER is an error return flag, which is 0 for success or non-zero if an error occurred.

4. **Linear solver specification**

The variable-order, variable-coefficient BDF method used by IDA involves the solution of linear systems related to the system Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial y'$. See Eq. (3.4). IDA presently includes five choices for the treatment of these systems, and the user of FIDA must call a routine with a specific name to make the desired choice.

[**S**] **Dense treatment of the linear system**

The user must make the call:

```
CALL FIDADENSE (NEQ, IER)
```

where NEQ is the size of the DAE system. The argument IER is an error return flag, which is 0 for success , -1 if a memory allocation failure occurred, or -2 for illegal input. As an option when using the DENSE linear solver, the user may supply a routine that computes a dense approximation of the system Jacobian. If supplied, it must have the following form:

```
 SUBROUTINE FIDADJAC (NEQ, T, Y, YP, R, DJAC, CJ, EWT, H,
&                     IPAR, RPAR, WK1, WK2, WK3, IER)
 DIMENSION Y(*), YP(*), R(*), EWT(*), DJAC(NEQ,*),
&          IPAR(*), RPAR(*), WK1(*), WK2(*), WK3(*)
```

This routine must compute the Jacobian and store it columnwise in DJAC. The vectors WK1, WK2, and WK3 of length NEQ are provided as work space for use in FIDADJAC. The input arguments T, Y, YP, R, and CJ are the current values of t, y, y', $F(t, y, y')$, and α, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDADJAC uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

If the FIDADJAC routine is provided, then, following the call to FIDADENSE, the user must make the call:

```
CALL FIDADENSESETJAC (FLAG, IER)
```

with FLAG $\neq 0$ to specify use of the user-supplied Jacobian approximation. The argument IER is an error return flag, which is 0 for success or non-zero if an error occurred.

Optional outputs specific to the DENSE case are listed in Table 6.2.

[**S**] **Band treatment of the linear system**

The user must make the call:

```
CALL FIDABAND (NEQ, MU, ML, IER)
```

The arguments are: MU, the upper half-bandwidth; ML, the lower half-bandwidth; and IER, an error return flag, which is 0 for success , -1 if a memory allocation failure occurred, or -2 in case an input has an illegal value.

As an option when using the BAND linear solver, the user may supply a routine that computes a band approximation of the system Jacobian. If supplied, it must have the following form:

```
 SUBROUTINE FIDABJAC(NEQ, MU, ML, MDIM, T, Y, YP, R, CJ, BJAC,
&                    EWT, H, IPAR, RPAR, WK1, WK2, WK3, IER)
 DIMENSION Y(*), YP(*), R(*), EWT(*), BJAC(MDIM,*),
&          IPAR(*), RPAR(*), WK1(*), WK2(*), WK3(*)
```

This routine must load the MDIM by NEQ array BJAC with the Jacobian matrix at the current (t, y, y') in band form. Store in BJAC(k, j) the Jacobian element $J_{i,j}$ with $k = i - j$+MU+1 ($k = 1 \cdots$ ML + MU + 1) and $j = 1 \cdots N$. The vectors WK1, WK2, and WK3 of length NEQ are provided as work space for use in FIDABJAC. The input arguments T, Y, YP, R, and CJ are the current values of t, y, y', $F(t, y, y')$, and α, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDABJAC uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

If the FIDABJAC routine is provided, then, following the call to FIDABAND, the user must make the call:

```
CALL FIDABANDSETJAC (FLAG, IER)
```

with FLAG $\neq 0$ to specify use of the user-supplied Jacobian approximation. The argument IER is an error return flag, which is 0 for success or non-zero if an error occurred.

Optional outputs specific to the BAND case are listed in Table 6.2.

[S][P] SPGMR treatment of the linear systems

For the Scaled Preconditioned GMRES solution of the linear systems, the user must make the call

```
CALL FIDASPGMR (MAXL, IGSTYPE, MAXRS, EPLIFAC, DQINCFAC, IER)
```

The arguments are as follows. MAXL is the maximum Krylov subspace dimension. IGSTYPE indicates the Gram-Schmidt process type: 1 for modified, or 2 for classical. MAXRS maximum number of restarts. EPLIFAC is the linear convergence tolerance factor. DQINCFAC is the optional increment factor used in the matrix-vector product Jv. For all the input arguments, a value of 0 or 0.0 indicates the default. IER is an error return flag, which is 0 to indicate success, -1 if a memory allocation failure occurred, or -2 to indicate an illegal input.

Optional outputs specific to the SPGMR case are listed in Table 6.2.

For descriptions of the relevant optional user-supplied routines, see **User-supplied routines for SPGMR/SPBCG/SPTFQMR** below.

[S][P] SPBCG treatment of the linear systems

For the Scaled Preconditioned Bi-CGStab solution of the linear systems, the user must make the call

```
CALL FIDASPBCG (MAXL, EPLIFAC, DQINCFAC, IER)
```

The arguments are as follows. MAXL is the maximum Krylov subspace dimension. EPLIFAC is the linear convergence tolerance factor. DQINCFAC is the optional increment factor used in the matrix-vector product Jv. For all the input arguments, a value of 0 or 0.0 indicates the default. IER is an error return flag, which is 0 to indicate success, -1 if a memory allocation failure occurred, or -2 to indicate an illegal input.

Optional outputs specific to the SPBCG case are listed in Table 6.2.

For descriptions of the relevant optional user-supplied routines, see **User-supplied routines for SPGMR/SPBCG/SPTFQMR** below.

[S][P] SPTFQMR treatment of the linear systems

For the Scaled Preconditioned Transpose-Free Quasi-Minimal Residual solution of the linear systems, the user must make the call

```
CALL FIDASPTFQMR (MAXL, EPLIFAC, DQINCFAC, IER)
```

The arguments are as follows. MAXL is the maximum Krylov subspace dimension. EPLIFAC is the linear convergence tolerance factor. DQINCFAC is the optional increment factor used in the matrix-vector product Jv. For all the input arguments, a value of 0 or 0.0 indicates the default. IER is an error return flag, which is 0 to indicate success, -1 if a memory allocation failure occurred, or -2 to indicate an illegal input.

Optional outputs specific to the SPTFQMR case are listed in Table 6.2.

For descriptions of the relevant optional user-supplied routines, see below.

[S][P] Functions used by SPGMR/SPBCG/SPTFQMR

An optional user-supplied routine, FIDAJTIMES, can be provided for Jacobian-vector products. If it is, then, following the call to FIDASPGMR, FIDASPBCG, or FIDASPTFQMR, the user must make the call:

```
CALL FIDASPILSSETJAC (FLAG, IER)
```

with FLAG $\neq 0$. The return flag IER is 0 if successful, or negative if a memory error occurred.

If preconditioning is to be done, then the user must call

```
CALL FIDASPILSSETPREC (FLAG, IER)
```

with FLAG $\neq 0$. The return flag IER is 0 if successful, or negative if a memory error occurred. In addition, the user must supply preconditioner routines FIDAPSET and FIDAPSOL.

[S][P] User-supplied routines for SPGMR/SPBCG/SPTFQMR

With treatment of the linear systems by any of the Krylov iterative solvers, there are three optional user-supplied routines — FIDAJTIMES, FIDAPSOL, and FIDAPSET. The specifications for these routines are given below.

As an option when using any of the Krylov iterative solvers, the user may supply a routine that computes the product of the system Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial y'$ and a given vector v. If supplied, it must have the following form:

```
 SUBROUTINE FIDAJTIMES(T, Y, YP, R, V, FJV, CJ, EWT, H,
&                      IPAR, RPAR, WK1, WK2, IER)
 DIMENSION Y(*), YP(*), R(*), V(*), FJV(*), EWT(*),
&          IPAR(*), RPAR(*), WK1(*), WK2(*)
```

This routine must compute the product vector Jv, where the vector v is stored in V, and store the product in FJV. On return, set IER = 0 if FIDAJTIMES was successful, and nonzero otherwise. The vectors W1K and WK2, of length NEQ, are provided as work space for use in FIDAJTIMES. The input arguments T, Y, YP, R, and CJ are the current values of t, y, y', $F(t, y, y')$, and α, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDAJTIMES uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

If preconditioning is to be included, the following routine must be supplied, for solution of the preconditioner linear system:

```
 SUBROUTINE FIDAPSOL(T, Y, YP, R, RV, ZV, CJ, DELTA, EWT,
&                    IPAR, RPAR, WK1, IER)
 DIMENSION Y(*), YP(*), R(*), RV(*), ZV(*), EWT(*),
&          IPAR(*), RPAR(*), WK1(*)
```

It must solve the preconditioner linear system $Pz = r$, where $r =$ RV is input, and store the solution z in ZV. Here P is the left preconditioner if LR=1 and the right preconditioner if LR=2. The input arguments T, Y, YP, R, and CJ are the current values of t, y, y', $F(t, y, y')$, and α, respectively. On return, set IER = 0 if FIDAPSOL was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred.

The arguments EWT and DELTA are input and provide the error weight array and a scalar tolerance, respectively, for use by FIDAPSOL if it uses an iterative method in its solution. In that case, the residual vector $\rho = r - Pz$ of the system should be made less than DELTA in weighted ℓ_2 norm, i.e. $\sqrt{\sum(\rho_i * \mathtt{EWT}[i])^2} <$ DELTA. The argument WK1 is a work array of length NEQ for use by this routine. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's preconditioner requires that any Jacobian-related data be evaluated or preprocessed, then the following routine is to be used for the evaluation and preprocessing of the preconditioner:

```
 SUBROUTINE FIDAPSET(T, Y, YP, R, CJ, EWT, H,
&                    IPAR, RPAR, WK1, WK2, WK3, IER)
 DIMENSION Y(*), YP(*), R(*), EWT(*),
&          IPAR(*), RPAR(*), WK1(*), WK2(*), WK3(*)
```

It must perform any evaluation of Jacobian-related data and preprocessing needed for the solution of the preconditioner linear systems by FIDAPSOL. The input arguments T, Y, YP, R, and CJ are the current values of t, y, y', $F(t, y, y')$, and α, respectively. On return, set IER = 0 if FIDAPSET was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDAPSET uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

If the user calls FIDASPILSSETPREC, the subroutine FIDAPSET must be provided, even if it is not needed and must return IER=0.

5. **Correct initial values**

Optionally, to correct the initial values y and/or y', make the call

```
CALL FIDACALCIC (ICOPT, TOUT1, IER)
```

(See §3.1 for details.) The arguments are as follows: ICOPT is 1 for initializing the algebraic components of y and differential components of y', or 2 for initializing all of y. IER is an error return flag, which is 0 for success, or negative for a failure (see IDACalcIC return values).

6. **Problem solution**

Carrying out the integration is accomplished by making calls as follows:

```
CALL FIDASOLVE (TOUT, T, Y, YP, ITASK, IER)
```

The arguments are as follows. TOUT specifies the next value of t at which a solution is desired (input). T is the value of t reached by the solver on output. Y is an array containing the computed solution vector y on output. YP is an array containing the computed solution vector y' on output. ITASK is a task indicator and should be set to 1 for normal mode (overshoot TOUT and interpolate), to 2 for one-step mode (return after each internal step taken), to 3 for normal mode with the additional tstop constraint, or to 4 for one-step mode with the additional constraint tstop. IER is a completion flag and will be set to a positive value upon successful return or to a negative value if an error occurred. These values correspond to the IDASolve returns (see §5.5.5 and §10.2). The current values of the optional outputs are available in IOUT and ROUT (see Table 6.2).

7. **Additional solution output**

After a successful return from FIDASOLVE, the routine FIDAGETSOL may be called to get interpolated values of y and y' for any value of t in the last internal step taken by IDA.

```
CALL FIDAGETSOL (T, Y, YP, IER)
```

where T is the input value of t at which solution derivative is desired, and Y and YP are arrays containing the computed vectors y and y' on return. The value T must lie between TCUR-HLAST and TCUR. The return flag IER is set to 0 upon successful return, or to a negative value to indicate an illegal input.

8. **Problem reinitialization**

   To re-initialize the IDA solver for the solution of a new problem of the same size as one already solved, make the following call:

   ```
   CALL FIDAREINIT (T0, Y0, YP0, IATOL, RTOL, ATOL, IER)
   ```

   The arguments have the same names and meanings as those of FIDAMALLOC. FIDAREINIT performs the same initializations as FIDAMALLOC, but does no memory allocation, using instead the existing internal memory created by the previous FIDAMALLOC call.

   Following this call, a call to specify the linear system solver must be made if the choice of linear solver is being changed. Otherwise, a call to reinitialize the linear solver last used may or may not be needed, depending on changes in the inputs to it.

   In the case of the BAND solver, for any change in the half-bandwidths, call FIDABAND as described above.

   In the case of SPGMR, for a change of inputs other than MAXL, make the call

   ```
   CALL FIDASPGMRREINIT (IGSTYPE, MAXRS, EPLIFAC, DQINCFAC, IER)
   ```

   which reinitializes SPGMR without reallocating its memory. The arguments have the same names and meanings as those of FIDASPGMR. If MAXL is being changed, then call FIDASPGMR.

   In the case of SPBCG, for a change in any inputs, make the call

   ```
   CALL FIDASPBCGREINIT (MAXL, EPLIFAC, DQINCFAC, IER)
   ```

   which reinitializes SPBCG without reallocating its memory. The arguments have the same names and meanings as those of FIDASPBCG.

   In the case of SPTFQMR, for a change in any inputs, make the call

   ```
   CALL FIDASPTFQMRREINIT (MAXL, EPLIFAC, DQINCFAC, IER)
   ```

   which reinitializes SPTFQMR without reallocating its memory. The arguments have the same names and meanings as those of FIDASPTFQMR.

9. **Memory deallocation**

   To free the internal memory created by the call to FIDAMALLOC, make the call

   ```
   CALL FIDAFREE
   ```

6.3 FIDA optional input and output

In order to keep the number of user-callable FIDA interface routines to a minimum, optional inputs to the IDA solver are passed through only three routines: FIDASETIIN for integer optional inputs, FIDASETRIN for real optional inputs, and FIDASETVIN for real vector (array) optional inputs. These functions should be called as follows:

Table 6.1: Keys for setting FIDA optional inputs

Integer optional inputs (FIDASETIIN)

Key	Optional input	Default value
MAX_ORD	Maximum LMM method order	5
MAX_NSTEPS	Maximum no. of internal steps before t_{out}	500
MAX_ERRFAIL	Maximum no. of error test failures	10
MAX_NITERS	Maximum no. of nonlinear iterations	4
MAX_CONVFAIL	Maximum no. of convergence failures	10
SUPPRESS_ALG	Suppress alg. vars. from error test (1 = TRUE)	0 (= FALSE)
MAX_NSTEPS_IC	Maximum no. of steps for IC calc.	5
MAX_NITERS_IC	Maximum no. of Newton iterations for IC calc.	10
MAX_NJE_IC	Maximum no. of Jac. evals fo IC calc.	4
LS_OFF_IC	Turn off line search (1 = TRUE)	0 (= FALSE)

Real optional inputs (FIDASETRIN)

Key	Optional input	Default value
INIT_STEP	Initial step size	estimated
MAX_STEP	Maximum absolute step size	∞
STOP_TIME	Value of t_{stop}	undefined
NLCONV_COEF	Coeff. in the nonlinear conv. test	0.33
NLCONV_COEF_IC	Coeff. in the nonlinear conv. test for IC calc.	0.0033
STEP_TOL_IC	Lower bound on Newton step for IC calc.	$\text{uround}^{2/3}$

Real vector optional inputs (FIDASETVIN)

Key	Optional input	Default value
ID_VEC	Differential/algebraic component types	undefined
CONSTR_VEC	Inequality constraints on solution	undefined

```
CALL FIDASETIIN(KEY, IVAL, IER)
CALL FIDASETRIN(KEY, RVAL, IER)
CALL FIDASETVIN(KEY, VVAL, IER)
```

where KEY is a quoted string indicating which optoinal input is set (see Table 6.1), IVAL is the input integer value, RVAL is the input real value (scalar), VVAL is the input real array, and IER is an integer return flag which is set to 0 on success and a negative value if a failure occurred.

When using FIDASETVIN to specify the variable types (KEY = 'ID_VEC') the components in the array VVAL must be 1.0 to indicate a differential variable, or 0.0 to indicate an algebraic variable. Note that this array is required only if FIDACALCIC is to be called with ICOPT = 1, or if algebraic variables are suppressed from the error test (indicated using FIDASETIIN with KEY = 'SUPPRESS_ALG'). When using FIDASETVIN to specify optional constraints on the solution vector (KEY = 'CONSTR_VEC') the components in the array VVAL should be one of −2.0, −1.0, 0.0, 1.0, or 2.0. See the description of IDASetConstraints (§5.5.6.1) for details.

The optional outputs from the IDA solver are accessed not through individual functions, but rather through a pair of arrays, IOUT (integer type) of dimension at least 21, and ROUT (real type) of dimension at least 6. These arrays are owned (and allocated) by the user and are passed as arguments to FIDAMALLOC. Table 6.2 lists the entries in these two arrays and specifies the optional variable as well as the IDA function which is actually called to extract the optional output.

For more details on the optional inputs and outputs, see §5.5.6 and §5.5.8.

In addition to the optional inputs communicated through FIDASET* calls and the optional outputs extracted from IOUT and ROUT, the following user-callable routines are available:

To reset the tolerances at any time, make the following call:

```
CALL FIDATOLREINIT (IATOL, RTOL, ATOL, IER)
```

Table 6.2: Description of the FIDA optional output arrays IOUT and ROUT

Integer output array IOUT

Index	Optional output	IDA function
IDA main solver		
1	LENRW	IDAGetWorkSpace
2	LENIW	IDAGetWorkSpace
3	NST	IDAGetNumSteps
4	NRE	IDAGetNumResEvals
5	NETF	IDAGetNumErrTestFails
6	NNCFAILS	IDAGetNonlinSolvConvFails
7	NNI	IDAGetNumNonlinSolvIters
8	NSETUPS	IDAGetNumLinSolvSetups
9	QLAST	IDAGetLastOrder
10	QCUR	IDAGetCurrentOrder
11	NBCKTRKOPS	IDAGetNumBacktrackOps
12	NGE	IDAGetNumGEvals
IDADENSE linear solver		
13	LENRWLS	IDADenseGetWorkSpace
14	LENIWLS	IDADenseGetWorkSpace
15	LS_FLAG	IDADenseGetLastFlag
16	NRELS	IDADenseGetNumResEvals
17	NJE	IDADenseGetNumJacEvals
IDABAND linear solver		
13	LENRWLS	IDABandGetWorkSpace
14	LENIWLS	IDABandGetWorkSpace
15	LS_FLAG	IDABandGetLastFlag
16	NRELS	IDABandGetNumResEvals
17	NJE	IDABandGetNumJacEvals
IDASPGMR, IDASPBCG, IDASPTFQMR linear solvers		
13	LENRWLS	IDASpilsGetWorkSpace
14	LENIWLS	IDASpilsGetWorkSpace
15	LS_FLAG	IDASpilsGetLastFlag
16	NRELS	IDASpilsGetNumResEvals
17	NJE	IDASpilsGetNumJtimesEvals
18	NPE	IDASpilsGetNumPrecEvals
19	NPS	IDASpilsGetNumPrecSolves
20	NLI	IDASpilsGetNumLinIters
21	NCFL	IDASpilsGetNumConvFails

Real output array ROUT

Index	Optional output	IDA function
1	H0_USED	IDAGetActualInitStep
2	HLAST	IDAGetLastStep
3	HCUR	IDAGetCurrentStep
4	TCUR	IDAGetCurrentTime
5	TOLFACT	IDAGetTolScaleFactor
6	UROUND	unit roundoff

The tolerance arguments have the same names and meanings as those of FIDAMALLOC. The error return flag IER is 0 if successful, and negative if there was a memory failure or illegal input.

To obtain the error weight array EWT, containing the multiplicative error weights used the WRMS norms, make the following call:

```
CALL FIDAGETERRWEIGHTS (EWT, IER)
```

This computes the EWT array, normally defined by Eq. (3.6). The array EWT, of length NEQ or NLOCAL, must already have been declared by the user. The error return flag IER is zero if successful, and negative if there was a memory error.

To obtain the estimated local errors, following a successful call to FIDASOLVE, make the following call:

```
CALL FIDAGETESTLOCALERR (ELE, IER)
```

This computes the ELE array of estimated local errors as of the last step taken. The array ELE must already have been declared by the user. The error return flag IER is zero if successful, and negative if there was a memory error.

6.4 Usage of the FIDAROOT interface to rootfinding

The FIDAROOT interface package allows programs written in FORTRAN to use the rootfinding feature of the IDA solver module. The user-callable functions in FIDAROOT, with the corresponding IDA functions, are as follows:

- FIDAROOTINIT interfaces to IDARootInit.
- FIDAROOTINFO interfaces to IDAGetRootInfo.
- FIDAROOTFREE interfaces to IDARootFree.

In order to use the rootfinding feature of IDA, the following call must be made, after calling FIDAMALLOC but prior to calling FIDASOLVE, to allocate and initialize memory for the FIDAROOT module:

```
CALL FIDAROOTINIT (NRTFN, IER)
```

The arguments are as follows: NRTFN is the number of root functions. IER is a return completion flag; its values are 0 for success, -1 if the IDA memory was NULL, and -14 if a memory allocation failed.

To specifiy the functions whose roots are to be found, the user must define the following routine:

```
SUBROUTINE FIDAROOTFN (T, Y, YP, G, IPAR, RPAR, IER)
DIMENSION Y(*), YP(*), G(*), IPAR(*), RPAR(*)
```

It must set the G array, of length NRTFN, with components $g_i(t, y, y')$, as a function of T $= t$ and the arrays Y $= y$ and YP $= y'$. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC. Set IER on 0 if successful, or on a non-zero value if an error occurred.

When making calls to FIDASOLVE to solve the DAE system, the occurrence of a root is flagged by the return value IER $= 2$. In that case, if NRTFN > 1, the functions g_i which were found to have a root can be identified by making the following call:

```
CALL FIDAROOTINFO (NRTFN, INFO, IER)
```

The arguments are as follows: NRTFN is the number of root functions. INFO is an integer array of length NRTFN with root information. IER is a return completion flag; its values are 0 for success, negative if there was a memory failure. The returned values of INFO(i) (i$= 1, \ldots,$ NRTFN) are 0 or 1, such that INFO(i) $= 1$ if $g_{\mathtt{i}}$ was found to have a root, and INFO(i) $= 0$ otherwise.

The total number of calls made to the root function FIDAROOTFN, denoted NGE, can be obtained from IOUT(12). If the FIDA/IDA memory block is reinitialized to solve a different problem via a call to FIDAREINIT, then the counter NGE is reset to zero.

To free the memory resources allocated by a prior call to FIDAROOTINIT make the following call:

```
CALL FIDAROOTFREE
```

See §5.7 for additional information on the rootfinding feature.

6.5 Usage of the FIDABBD interface to IDABBDPRE

The FIDABBD interface sub-module is a package of C functions which, as part of the FIDA interface module, support the use of the IDA solver with the parallel NVECTOR_PARALLEL module, in a combination of any of the Krylov iterative solver modules with the IDABBDPRE preconditioner module (see §5.8).

The user-callable functions in this package, with the corresponding IDA and IDABBDPRE functions, are as follows:

- `FIDABBDINIT` interfaces to `IDABBDPrecAlloc`.
- `FIDABBDSPGMR` interfaces to `IDABBDSpgmr` and SPGMR optional input functions.
- `FIDABBDSPBCG` interfaces to `IDABBDSpbcg` and SPBCG optional input functions.
- `FIDABBDSPTFQMR` interfaces to `IDABBDSptfqmr` and SPTFQMR optional input functions.
- `FIDABBDREINIT` interfaces to `IDABBDPrecReInit`.
- `FIDABBDOPT` interfaces to IDABBDPRE optional output functions.
- `FIDABBDFREE` interfaces to `IDABBDPrecFree`.

In addition to the FORTRAN residual function `FIDARESFUN`, the user-supplied functions used by this package, are listed below, each with the corresponding interface function which calls it (and its type within IDABBDPRE or IDA):

FIDABBD routine (FORTRAN)	IDA function (C)	IDA function type
FIDAGLOCFN	FIDAgloc	IDABBDLocalFn
FIDACOMMFN	FIDAcfn	IDABBDCommFn
FIDAJTIMES	FIDAJtimes	IDASpilsJacTimesVecFn

As with the rest of the FIDA routines, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program. Additionally, based on flags discussed above in §6.1, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fidabbd.h`.

The following is a summary of the usage of this module. Steps that are unchanged from the main program described in §6.2 are grayed-out.

1. **Residual function specification**
2. **NVECTOR module initialization**
3. **Problem specification**
4. **Linear solver specification**

   To initialize the IDABBDPRE preconditioner, make the following call:

   ```
   CALL FIDABBDINIT (NLOCAL, MUDQ, MLDQ, MU, ML, DQRELY, IER)
   ```

   The arguments are as follows. `NLOCAL` is the local size of vectors on this processor. `MUDQ` and `MLDQ` are the upper and lower half-bandwidths to be used in the computation of the local Jacobian blocks by difference quotients. These may be smaller than the true half-bandwidths of the Jacobian of the local block of G, when smaller values may provide greater efficiency. `MU` and `ML` are the upper

and lower half-bandwidths of the band matrix that is retained as an approximation of the local Jacobian block. These may be smaller than MUDQ and MLDQ. DQRELY is the relative increment factor in y for difference quotients (optional). A value of 0.0 indicates the default, $\sqrt{\text{unit roundoff}}$. IER is a return completion flag. A value of 0 indicates success, while a value of -1 indicates that a memory failure occurred or that an input had an illegal value.

To specify the SPGMR linear system solver and use the IDABBDPRE preconditioner, make the following call:

```
CALL FIDABBDSPGMR (MAXL, IGSTYPE, MAXRS, EPLIFAC, DQINCFAC, IER)
```

Its arguments are the same as those of FIDASPGMR (see step 4 in §6.2).

To specify the SPBCG linear system solver and use the IDABBDPRE preconditioner, make the following call:

```
CALL FIDABBDSPBCG (MAXL, EPLIFAC, DQINCFAC, IER)
```

Its arguments are the same as those of FIDASPBCG (see step 4 in §6.2).

To specify the SPTFQMR linear system solver and use the IDABBDPRE preconditioner, make the following call:

```
CALL FIDABBDSPTFQMR (MAXL, EPLIFAC, DQINCFAC, IER)
```

Its arguments are the same as those of FIDASPTFQMR (see step 4 in §6.2).

Optionally, to specify that SPGMR, SPBCG, or SPTFQMR should use the supplied FIDAJTIMES, make the call

```
CALL FIDASPILSSETJAC (FLAG, IER)
```

with FLAG $\neq 0$ (see step 4 in §6.2 for details).

5. **Problem solution**

6. IDABBDPRE **Optional outputs**

Optional outputs specific to the SPGMR, SPBCG, or SPTFQMR solver are listed in Table 6.2. To obtain the optional outputs associated with the IDABBDPRE module, make the following call:

```
CALL FIDABBDOPT (LENRWBBD, LENIWBBD, NGEBBD)
```

The arguments returned are as follows. LENRWBBD is the length of real preconditioner work space, in realtype words. LENIWBBD is the length of integer preconditioner work space, in integer words. Both of these sizes are local to the current processor. NGEBBD is the number of $G(t, y, y')$ evaluations (calls to FIDALOCFN) so far.

7. **Problem reinitialization**

If a sequence of problems of the same size is being solved using the SPGMR, SPBCG, or SPTFQMR linear solver in combination with the IDABBDPRE preconditioner, then the IDA package can be reinitialized for the second and subsequent problems by calling FIDAREINIT, following which a call to FIDABBDINIT may or may not be needed. If the input arguments are the same, no FIDABBDINIT call is needed. If there is a change in input arguments other than MU, ML, or MAXL, then the user program should make the call

```
CALL FIDABBDREINIT (NLOCAL, MUDQ, MLDQ, DQRELY, IER)
```

This reinitializes the IDABBDPRE preconditioner, but without reallocating its memory. The arguments of the FIDABBDREINIT routine have the same names and meanings as those of FIDABBDINIT. If the value of MU or ML is being changed, then a call to FIDABBDINIT must be made. Finally, if MAXL is being changed, then a call to FIDABBDSPGMR, FIDABBDSPBCG, or FIDASPTFQMR must be made; in this case the linear solver memory is reallocated.

8. **Memory deallocation**

To free the internal memory created by the call to FIDABBDINIT, before calling FIDAFREE, the user must call

```
CALL FIDABBDFREE
```

9. **User-supplied routines**

The following two routines must be supplied for use with the IDABBDPRE module:

```
SUBROUTINE FIDAGLOCFN (NLOC, T, YLOC, YPLOC, GLOC, IPAR, RPAR, IER)
DIMENSION YLOC(*), YPLOC(*), GLOC(*), IPAR(*), RPAR(*)
```

This routine is to evaluate the function $G(t, y, y')$ approximating F (possibly identical to F), in terms of T $= t$, and the arrays YLOC and YPLOC (of length NLOC), which are the sub-vectors of y and y' local to this processor. The resulting (local) sub-vector is to be stored in the array GLOC. IER is a return flag that should be set to 0 if successful, to 1 (for a recoverable error), or to -1 (for a non-recoverable error). The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

```
SUBROUTINE FIDACOMMFN (NLOC, T, YLOC, YPLOC, IPAR, RPAR, IER)
DIMENSION YLOC(*), YPLOC(*), IPAR(*), RPAR(*)
```

This routine is to perform the inter-processor communication necessary for the FIDAGLOCFN routine. Each call to FIDACOMMFN is preceded by a call to the residual routine FIDARESFUN with the same arguments T, YLOC, and YPLOC. Thus FIDACOMMFN can omit any communications done by FIDARESFUN if relevant to the evaluation of GLOC. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC. IER is a return flag that should be set to 0 if successful, to 1 (for a recoverable error), or to -1 (for a non-recoverable error).

The subroutine FIDACOMMFN must be supplied even if it is empty and it must return IER=0.

Optionally, the user can supply a routine FIDAJTIMES for the evaluation of Jacobian-vector products, as described above in step 4 in §6.2.

Chapter 7

Description of the NVECTOR module

The SUNDIALS solvers are written in a data-independent manner. They all operate on generic vectors (of type `N_Vector`) through a set of operations defined by the particular NVECTOR implementation. Users can provide their own specific implementation of the NVECTOR module or use one of two provided within SUNDIALS, a serial and an MPI parallel implementations.

The generic `N_Vector` type is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the vector, and an *ops* field pointing to a structure with generic vector operations. The type `N_Vector` is defined as

```
typedef struct _generic_N_Vector *N_Vector;

struct _generic_N_Vector {
    void *content;
    struct _generic_N_Vector_Ops *ops;
};
```

The `_generic_N_Vector_Ops` structure is essentially a list of pointers to the various actual vector operations, and is defined as

```
struct _generic_N_Vector_Ops {
  N_Vector    (*nvclone)(N_Vector);
  N_Vector    (*nvcloneempty)(N_Vector);
  void        (*nvdestroy)(N_Vector);
  void        (*nvspace)(N_Vector, long int *, long int *);
  realtype*   (*nvgetarraypointer)(N_Vector);
  void        (*nvsetarraypointer)(realtype *, N_Vector);
  void        (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
  void        (*nvconst)(realtype, N_Vector);
  void        (*nvprod)(N_Vector, N_Vector, N_Vector);
  void        (*nvdiv)(N_Vector, N_Vector, N_Vector);
  void        (*nvscale)(realtype, N_Vector, N_Vector);
  void        (*nvabs)(N_Vector, N_Vector);
  void        (*nvinv)(N_Vector, N_Vector);
  void        (*nvaddconst)(N_Vector, realtype, N_Vector);
  realtype    (*nvdotprod)(N_Vector, N_Vector);
  realtype    (*nvmaxnorm)(N_Vector);
  realtype    (*nvwrmsnorm)(N_Vector, N_Vector);
  realtype    (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
  realtype    (*nvmin)(N_Vector);
```

```
  realtype    (*nvwl2norm)(N_Vector, N_Vector);
  realtype    (*nvl1norm)(N_Vector);
  void        (*nvcompare)(realtype, N_Vector, N_Vector);
  booleantype (*nvinvtest)(N_Vector, N_Vector);
  booleantype (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
  realtype    (*nvminquotient)(N_Vector, N_Vector);
};
```

The generic NVECTOR module defines and implements the vector operations acting on `N_Vector`. These routines are nothing but wrappers for the vector operations defined by a particular NVECTOR implementation, which are accessed through the *ops* field of the `N_Vector` structure. To illustrate this point we show below the implementation of a typical vector operation from the generic NVECTOR module, namely `N_VScale`, which performs the scaling of a vector `x` by a scalar `c`:

```
void N_VScale(realtype c, N_Vector x, N_Vector z)
{
   z->ops->nvscale(c, x, z);
}
```

Table 7.1 contains a complete list of all vector operations defined by the generic NVECTOR module.

Finally, note that the generic NVECTOR module defines the functions `N_VCloneVectorArray` and `N_VCloneEmptyVectorArray`. Both functions create (by cloning) an array of `count` variables of type `N_Vector`, each of the same type as an existing `N_Vector`. Their prototypes are

```
N_Vector *N_VCloneVectorArray(int count, N_Vector w);
N_Vector *N_VCloneEmptyVectorArray(int count, N_Vector w);
```

and their definitions are based on the implementation-specific `N_VClone` and `N_VCloneEmpty` operations, respectively.

An array of variables of type `N_Vector` can be destroyed by calling `N_VDestroyVectorArray`, whose prototype is

```
void N_VDestroyVectorArray(N_Vector *vs, int count);
```

and whose definition is based on the implementation-specific `N_VDestroy` operation.

A particular implementation of the NVECTOR module must:

- Specify the *content* field of `N_Vector`.
- Define and implement the vector operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one NVECTOR module (each with different `N_Vector` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free an `N_Vector` with the new *content* field and with *ops* pointing to the new vector operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined `N_Vector` (e.g., a routine to print the content for debugging purposes).
- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the *content* field of the newly defined `N_Vector`.

Table 7.1: Description of the NVECTOR operations

Name	Usage and Description
N_VClone	`v = N_VClone(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not copy the vector, but rather allocates storage for the new vector.
N_VCloneEmpty	`v = N_VCloneEmpty(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not allocate storage for the data array.
N_VDestroy	`N_VDestroy(v);` Destroys the `N_Vector v` and frees memory allocated for its internal data.
N_VSpace	`N_VSpace(nvSpec, &lrw, &liw);` Returns storage requirements for one `N_Vector`. `lrw` contains the number of realtype words and `liw` contains the number of integer words.
N_VGetArrayPointer	`vdata = N_VGetArrayPointer(v);` Returns a pointer to a `realtype` array from the `N_Vector v`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype`. This routine is only used in the solver-specific interfaces to the dense and banded linear solvers, as well as the interfaces to the banded preconditioners provided with SUNDIALS.
N_VSetArrayPointer	`N_VSetArrayPointer(vdata, v);` Overwrites the data in an `N_Vector` with a given array of `realtype`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype`. This routine is only used in the interfaces to the dense linear solver.
N_VLinearSum	`N_VLinearSum(a, x, b, y, z);` Performs the operation $z = ax + by$, where a and b are scalars and x and y are of type `N_Vector`: $z_i = ax_i + by_i$, $i = 0, \ldots, n-1$.
N_VConst	`N_VConst(c, z);` Sets all components of the `N_Vector z` to `c`: $z_i = c$, $i = 0, \ldots, n-1$.
N_VProd	`N_VProd(x, y, z);` Sets the `N_Vector z` to be the component-wise product of the `N_Vector` inputs `x` and `y`: $z_i = x_i y_i$, $i = 0, \ldots, n-1$.
N_VDiv	`N_VDiv(x, y, z);` Sets the `N_Vector z` to be the component-wise ratio of the `N_Vector` inputs `x` and `y`: $z_i = x_i/y_i$, $i = 0, \ldots, n-1$. The y_i may not be tested for 0 values. It should only be called with an `x` that is guaranteed to have all nonzero components.

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Name	Usage and Description
N_VScale	`N_VScale(c, x, z);` Scales the `N_Vector x` by the scalar `c` and returns the result in `z`: $z_i = cx_i$, $i = 0, \ldots, n-1$.
N_VAbs	`N_VAbs(x, z);` Sets the components of the `N_Vector z` to be the absolute values of the components of the `N_Vector x`: $y_i = \lvert x_i \rvert$, $i = 0, \ldots, n-1$.
N_VInv	`N_VInv(x, z);` Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine may not check for division by 0. It should be called only with an `x` which is guaranteed to have all nonzero components.
N_VAddConst	`N_VAddConst(x, b, z);` Adds the scalar `b` to all components of `x` and returns the result in the `N_Vector z`: $z_i = x_i + b$, $i = 0, \ldots, n-1$.
N_VDotProd	`d = N_VDotProd(x, y);` Returns the value of the ordinary dot product of `x` and `y`: $d = \sum_{i=0}^{n-1} x_i y_i$.
N_VMaxNorm	`m = N_VMaxNorm(x);` Returns the maximum norm of the `N_Vector x`: $m = \max_i \lvert x_i \rvert$.
N_VWrmsNorm	`m = N_VWrmsNorm(x, w)` Returns the weighted root-mean-square norm of the `N_Vector x` with weight vector `w`: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i)^2\right)/n}$.
N_VWrmsNormMask	`m = N_VWrmsNormMask(x, w, id);` Returns the weighted root mean square norm of the `N_Vector x` with weight vector `w` built using only the elements of `x` corresponding to nonzero elements of the `N_Vector id`: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i \mathrm{sign}(id_i))^2\right)/n}$.
N_VMin	`m = N_VMin(x);` Returns the smallest element of the `N_Vector x`: $m = \min_i x_i$.
N_VWL2Norm	`m = N_VWL2Norm(x, w);` Returns the weighted Euclidean ℓ_2 norm of the `N_Vector x` with weight vector `w`: $m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}$.
N_VL1Norm	`m = N_VL1Norm(x);` Returns the ℓ_1 norm of the `N_Vector x`: $m = \sum_{i=0}^{n-1} \lvert x_i \rvert$.
N_VCompare	`N_VCompare(c, x, z);` Compares the components of the `N_Vector x` to the scalar `c` and returns an `N_Vector z` such that: $z_i = 1.0$ if $\lvert x_i \rvert \geq c$ and $z_i = 0.0$ otherwise.

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Name	Usage and Description
N_VInvTest	`t = N_VInvTest(x, z);` Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`, with prior testing for zero values: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine returns `TRUE` if all components of `x` are nonzero (successful inversion) and returns `FALSE` otherwise.
N_VConstrMask	`t = N_VConstrMask(c, x, m);` Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \geq 0$ if $c_i = 1$, $x_i \leq 0$ 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 `FALSE` if any element failed the constraint test, `TRUE` 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.
N_VMinQuotient	`minq = N_VMinQuotient(num, denom);` This routine returns the minimum of the quotients obtained by termwise dividing $\texttt{num}_i$ by $\texttt{denom}_i$. 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.

7.1 The NVECTOR_SERIAL implementation

The serial implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_SERIAL, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, and a boolean flag *own_data* which specifies the ownership of *data*.

```
struct _N_VectorContent_Serial {
  long int length;
  booleantype own_data;
  realtype *data;
};
```

The following five macros are provided to access the content of an NVECTOR_SERIAL vector. The suffix `_S` in the names denotes serial version.

- `NV_CONTENT_S`

  This routine gives access to the contents of the serial vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_S(v)` sets `v_cont` to be a pointer to the serial `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
  ```

- `NV_OWN_DATA_S`, `NV_DATA_S`, `NV_LENGTH_S`

  These macros give individual access to the parts of the content of a serial `N_Vector`.

  The assignment `v_data = NV_DATA_S(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_S(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_len = NV_LENGTH_S(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_S(v) = len_v` sets the length of `v` to be `len_v`.

Implementation:

```
#define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )
```

```
#define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )
```

```
#define NV_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
```

- `NV_Ith_S`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_S(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_S(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_S(v,i) ( NV_DATA_S(v)[i] )
  ```

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Table 7.1. Their names are obtained from those in Table 7.1 by appending the suffix `_Serial`. The module NVECTOR_SERIAL provides the following additional user-callable routines:

- `N_VNew_Serial`

  This function creates and allocates memory for a serial `N_Vector`. Its only argument is the vector length.

  ```
  N_Vector N_VNew_Serial(long int vec_length);
  ```

- `N_VNewEmpty_Serial`

  This function creates a new serial `N_Vector` with an empty (`NULL`) data array.

  ```
  N_Vector N_VNewEmpty_Serial(long int vec_length);
  ```

- `N_VMake_Serial`

  This function creates and allocates memory for a serial vector with user-provided data array.

  ```
  N_Vector N_VMake_Serial(long int vec_length, realtype *v_data);
  ```

- `N_VCloneVectorArray_Serial`

  This function creates (by cloning) an array of `count` serial vectors.

  ```
  N_Vector *N_VCloneVectorArray_Serial(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Serial`

  This function creates (by cloning) an array of `count` serial vectors, each with an empty (`NULL`) data array.

  ```
  N_Vector *N_VCloneVectorArrayEmpty_Serial(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_Serial`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Serial` or with `N_VCloneVectorArrayEmpty_Serial`.

  ```
  void N_VDestroyVectorArray_Serial(N_Vector *vs, int count);
  ```

- `N_VPrint_Serial`

  This function prints the content of a serial vector to `stdout`.

  ```
  void N_VPrint_Serial(N_Vector v);
  ```

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_S(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_S(v,i)` within the loop.
- `N_VNewEmpty_Serial`, `N_VMake_Serial`, and `N_VCloneVectorArrayEmpty_Serial` set the field *own_data* = `FALSE`. `N_VDestroy_Serial` and `N_VDestroyVectorArray_Serial` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `FALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_SERIAL implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.2 The NVECTOR_PARALLEL implementation

The parallel implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_PARALLEL, defines the *content* field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the beginning of a contiguous local data array, an MPI communicator, an a boolean flag *own_data* indicating ownership of the data array *data*.

```
struct _N_VectorContent_Parallel {
  long int local_length;
  long int global_length;
  booleantype own_data;
  realtype *data;
  MPI_Comm comm;
};
```

The following seven macros are provided to access the content of a NVECTOR_PARALLEL vector. The suffix `_P` in the names denotes parallel version.

- `NV_CONTENT_P`

  This macro gives access to the contents of the parallel vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_P(v)` sets `v_cont` to be a pointer to the `N_Vector` content structure of type `struct _N_VectorParallelContent`.

  Implementation:

  ```
  #define NV_CONTENT_P(v) ( (N_VectorContent_Parallel)(v->content) )
  ```

- `NV_OWN_DATA_P`, `NV_DATA_P`, `NV_LOCLENGTH_P`, `NV_GLOBLENGTH_P`

  These macros give individual access to the parts of the content of a parallel `N_Vector`.

  The assignment `v_data = NV_DATA_P(v)` sets `v_data` to be a pointer to the first component of the local data for the `N_Vector v`. The assignment `NV_DATA_P(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_llen = NV_LOCLENGTH_P(v)` sets `v_llen` to be the length of the local part of `v`. The call `NV_LENGTH_P(v) = llen_v` sets the local length of `v` to be `llen_v`.

  The assignment `v_glen = NV_GLOBLENGTH_P(v)` sets `v_glen` to be the global length of the vector `v`. The call `NV_GLOBLENGTH_P(v) = glen_v` sets the global length of `v` to be `glen_v`.

  Implementation:

  ```
  #define NV_OWN_DATA_P(v)    ( NV_CONTENT_P(v)->own_data )
  #define NV_DATA_P(v)        ( NV_CONTENT_P(v)->data )
  ```

```
#define NV_LOCLENGTH_P(v)  ( NV_CONTENT_P(v)->local_length )
#define NV_GLOBLENGTH_P(v) ( NV_CONTENT_P(v)->global_length )
```

- `NV_COMM_P`

  This macro provides access to the MPI communicator used by the NVECTOR_PARALLEL vectors.

  Implementation:

  ```
  #define NV_COMM_P(v) ( NV_CONTENT_P(v)->comm )
  ```

- `NV_Ith_P`

  This macro gives access to the individual components of the local data array of an `N_Vector`.

  The assignment `r = NV_Ith_P(v,i)` sets `r` to be the value of the `i`-th component of the local part of `v`. The assignment `NV_Ith_P(v,i) = r` sets the value of the `i`-th component of the local part of `v` to be `r`.

  Here i ranges from 0 to $n-1$, where n is the local length.

  Implementation:

  ```
  #define NV_Ith_P(v,i) ( NV_DATA_P(v)[i] )
  ```

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Table 7.1 Their names are obtained from those in Table 7.1 by appending the suffix `_Parallel`. The module NVECTOR_PARALLEL provides the following additional user-callable routines:

- `N_VNew_Parallel`

  This function creates and allocates memory for a parallel vector.

  ```
  N_Vector N_VNew_Parallel(MPI_Comm comm,
                           long int local_length,
                           long int global_length);
  ```

- `N_VNewEmpty_Parallel`

  This function creates a new parallel `N_Vector` with an empty (`NULL`) data array.

  ```
  N_Vector N_VNewEmpty_Parallel(MPI_Comm comm,
                                long int local_length,
                                long int global_length);
  ```

- `N_VMake_Parallel`

  This function creates and allocates memory for a parallel vector with user-provided data array.

  ```
  N_Vector N_VMake_Parallel(MPI_Comm comm,
                            long int local_length,
                            long int global_length,
                            realtype *v_data);
  ```

- `N_VCloneVectorArray_Parallel`

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

  ```
  N_Vector *N_VCloneVectorArray_Parallel(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Parallel`

  This function creates (by cloning) an array of `count` parallel vectors, each with an empty (`NULL`) data array.

```
N_Vector *N_VCloneVectorArrayEmpty_Parallel(int count, N_Vector w);
```

- `N_VDestroyVectorArray_Parallel`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Parallel` or with `N_VCloneVectorArrayEmpty_Parallel`.

  ```
  void N_VDestroyVectorArray_Parallel(N_Vector *vs, int count);
  ```

- `N_VPrint_Parallel`

  This function prints the content of a parallel vector to stdout.

  ```
  void N_VPrint_Parallel(N_Vector v);
  ```

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the local component array via `v_data = NV_DATA_P(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_P(v,i)` within the loop.

- `N_VNewEmpty_Parallel`, `N_VMake_Parallel`, and `N_VCloneVectorArrayEmpty_Parallel` set the field *own_data* = `FALSE`. `N_VDestroy_Parallel` and `N_VDestroyVectorArray_Parallel` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `FALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PARALLEL implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.3 NVECTOR functions used by IDA

In Table 7.2 below, we list the vector functions in the NVECTOR module used by the IDA package. The table also shows, for each function, which of the code modules uses the function. The IDA column shows function usage within the main integrator module, while the remaining five columns show function usage within each of the five IDA linear solvers (IDASPILS stands for any of IDASPGMR, IDASPBCG, or IDASPTFQMR), the IDABBDPRE preconditioner module, and the FIDA module.

There is one subtlety in the IDASPILS column hidden by the table, explained here for the case of the IDASPGMR module). The `N_VDotProd` function is called both within the implementation file `ida_spgmr.c` for the IDASPGMR solver and within the implementation files `sundials_spgmr.c` and `sundials_iterative.c` for the generic SPGMR solver upon which the IDASPGMR solver is implemented. Also, although `N_VDiv` and `N_VProd` are not called within the implementation file `ida_spgmr.c`, they are called within the implementation file `sundials_spgmr.c` and so are required by the IDASPGMR solver module. This issue does not arise for the direct IDA linear solvers because the generic DENSE and BAND solvers (used in the implementation of IDADENSE and IDABAND) do not make calls to any vector functions.

Of the functions listed in Table 7.1, `N_VWL2Norm`, `N_VL1Norm`, `N_VCloneEmpty`, and `N_VInvTest` are *not* used by IDA. Therefore a user-supplied NVECTOR module for IDA could omit these four functions.

Table 7.2: List of vector functions usage by IDA code modules

	IDA	IDADENSE	IDABAND	IDASPILS	IDABBDPRE	FIDA
N_VClone	✓			✓	✓	
N_VDestroy	✓			✓	✓	
N_VSpace	✓					
N_VGetArrayPointer		✓	✓		✓	✓
N_VSetArrayPointer		✓				✓
N_VLinearSum	✓	✓		✓		
N_VConst	✓			✓		
N_VProd	✓			✓		
N_VDiv	✓			✓		
N_VScale	✓	✓	✓	✓	✓	
N_VAbs	✓					
N_VInv	✓					
N_VAddConst	✓					
N_VDotProd				✓		
N_VMaxNorm	✓					
N_VWrmsNorm	✓					
N_VMin	✓					
N_VMinQuotient	✓					
N_VConstrMask	✓					
N_VWrmsNormMask	✓					
N_VCompare	✓					

Chapter 8

Providing Alternate Linear Solver Modules

The central IDA module interfaces with the linear solver module to be used by way of calls to five routines. These are denoted here by `linit`, `lsetup`, `lsolve`, `lperf`, and `lfree`. Briefly, their purposes are as follows:

- `linit`: initialize and allocate memory specific to the linear solver;
- `lsetup`: evaluate and preprocess the Jacobian or preconditioner;
- `lsolve`: solve the linear system;
- `lperf`: monitor performance and issue warnings;
- `lfree`: free the linear solver memory.

A linear solver module must also provide a user-callable specification routine (like those described in §5.5.3) which will attach the above five routines to the main IDA memory block. The IDA memory block is a structure defined in the header file `ida_impl.h`. A pointer to such a structure is defined as the type `IDAMem`. The five fields in a `IDAMem` structure that must point to the linear solver's functions are `ida_linit`, `ida_lsetup`, `ida_lsolve`, `ida_lperf`, and `ida_lfree`, respectively. Note that of the four interface routines, only the `lsolve` routine is required. The `lfree` routine must be provided only if the solver specification routine makes any memory allocation. For consistency with the existing IDA linear solver modules, we recommend that the return value of the specification function be 0 for a successful return or a negative value if an error occurs (the pointer to the main IDA memory block is `NULL`, an input is illegal, the NVECTOR implementation is not compatible, a memory allocation fails, etc.)

To facilitate data exchange between the five interface functions, the field `ida_lmem` in the IDA memory block can be used to attach a linear solver-specific memory block.

These five routines, which interface between IDA and the linear solver module, necessarily have fixed call sequences. Thus a user wishing to implement another linear solver within the IDA package must adhere to this set of interfaces. The following is a complete description of the call list for each of these routines. Note that the call list of each routine includes a pointer to the main IDA memory block, by which the routine can access various data related to the IDA solution. The contents of this memory block are given in the file `ida.h` (but not reproduced here, for the sake of space).

8.1 Initialization function

The type definition of `linit` is

`linit`

Definition `int (*linit)(IDAMem IDA_mem);`

Purpose The purpose of `linit` is to complete initializations for a specific linear solver, such as counters and statistics.

Arguments `IDA_mem` is the IDA memory pointer of type `IDAMem`.

Return value An `linit` function should return 0 if it has successfully initialized the IDA linear solver and a negative value otherwise.

8.2 Setup routine

The type definition of `lsetup` is

`lsetup`

Definition
```
int (*lsetup)(IDAMem IDA_mem, N_Vector yyp, N_Vector ypp,
              N_Vector resp,
              N_Vector vtemp1, N_Vector vtemp2, N_Vector vtemp3);
```

Purpose The job of `lsetup` is to prepare the linear solver for subsequent calls to `lsolve`. It may re-compute Jacobian-related data if it deems necessary.

Arguments
- `IDA_mem` is the IDA memory pointer of type `IDAMem`.
- `yyp` is the predicted y vector for the current IDA internal step.
- `ypp` is the predicted y' vector for the current IDA internal step.
- `resp` is the value of the residual function at `yyp` and `ypp`, i.e. $F(t_n, y_{pred}, y'_{pred})$.
- `vtemp1`
- `vtemp2`
- `vtemp3` are temporary variables of type `N_Vector` provided for use by `lsetup`.

Return value The `lsetup` routine should return `0` if successful, a positive value for a recoverable error, and a negative value for an unrecoverable error.

8.3 Solve routine

The type definition of `lsolve` is

`lsolve`

Definition
```
int (*lsolve)(IDAMem IDA_mem, N_Vector b, N_Vector weight,
              N_Vector ycur, N_Vector ypcur, N_Vector rescur);
```

Purpose The routine `lsolve` must solve the linear equation $Mx = b$, where M is some approximation to $J = \partial F/\partial y + c_j \partial F/\partial y'$ (see Eqn. (3.5)), and the right-hand side vector b is input.

Arguments
- `IDA_mem` is the IDA memory pointer of type `IDAMem`.
- `b` is the right-hand side vector b. The solution is to be returned in the vector `b`.
- `weight` is a vector that contains the error weights. These are the W_i of (3.6).
- `ycur` is a vector that contains the solver's current approximation to $y(t_n)$.
- `ypcur` is a vector that contains the solver's current approximation to $y'(t_n)$.
- `rescur` is a vector that contains $F(t_n, y_{cur}, y'_{cur})$.

Return value `lsolve` returns a positive value for a recoverable error and a negative value for an unrecoverable error. Success is indicated by a `0` return value.

8.4 Performance monitoring routine

The type definition of `lperf` is

`lperf`

Definition `int (*lperf)(IDAMem IDA_mem, int perftask);`

Purpose The routine `lperf` is to monitor the performance of the linear solver.

Arguments `IDA_mem` is the IDA memory pointer of type `IDAMem`.

`perftask` is a task flag. `perftask` = 0 means initialize needed counters. `perftask` = 1 means evaluate performance and issue warnings if needed.

Return value The `lperf` return value is ignored.

8.5 Memory deallocation routine

The type definition of `lfree` is

`lfree`

Definition `void (*lfree)(IDAMem IDA_mem);`

Purpose The routine `lfree` should free up any memory allocated by the linear solver.

Arguments The argument `IDa_mem` is the IDA memory pointer of type `IDAMem`.

Return value This routine has no return value.

Notes This routine is called once a problem has been completed and the linear solver is no longer needed.

Chapter 9

Generic Linear Solvers in SUNDIALS

In this section, we describe five generic linear solver code modules that are included in IDA, but which are of potential use as generic packages in themselves, either in conjunction with the use of IDA or separately. These modules are:

- The DENSE matrix package, which includes the matrix type `DenseMat`, macros and functions for `DenseMat` matrices, and functions for small dense matrices treated as simple array types.
- The BAND matrix package, which includes the matrix type `BandMat`, macros and functions for `BandMat` matrices.
- The SPGMR package, which includes a solver for the scaled preconditioned GMRES method.
- The SPBCG package, which includes a solver for the scaled preconditioned Bi-CGStab method.
- The SPTFQMR package, which includes a solver for the scaled preconditioned TFQMR method.

For reasons related to installation, the names of the files involved in these generic solvers begin with the prefix `sundials_`. But despite this, each of the solvers is in fact generic, in that it is usable completely independently of SUNDIALS.

For the sake of space, the functions for `DenseMat` and `BandMat` matrices and the functions in SPGMR, SPBCG, and SPTFQMR are only summarized briefly, since they are less likely to be of direct use in connection with IDA. The functions for small dense matrices are fully described, because we expect that they will be useful in the implementation of preconditioners used with the combination of IDA and the IDASPGMR, IDASPBCG, or IDASPTFQMR solver.

9.1 The DENSE module

Relative to the SUNDIALS *srcdir*, the files comprising the DENSE generic linear solver are as follows:

- header files (located in *srcdir*`/include/sundials`)
  `sundials_dense.h` `sundials_smalldense.h`
  `sundials_types.h` `sundials_math.h` `sundials_config.h`
- source files (located in *srcdir*`/src/sundials`)
  `sundials_dense.c` `sundials_smalldense.c` `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are relevant to the DENSE package by itself (see §2.4 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```
- (optional) use of generic math functions: `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the `ABS` macro and `RAbs` function.

The eight files listed above can be extracted from the SUNDIALS *srcdir* and compiled by themselves into a DENSE library or into a larger user code.

9.1.1 Type DenseMat

The type `DenseMat` is defined to be a pointer to a structure with the number of rows, number of columns, and a data field:

```
typedef struct {
  long int M;
  long int N;
  realtype  **data;
} *DenseMat;
```

The M and N fields indicates the number of columns and rows, respectively, of a dense matrix, while the *data* field is a two dimensional array used for component storage. The elements of a dense matrix are stored columnwise (i.e columns are stored one on top of the other in memory). If `A` is of type `DenseMat`, then the (`i`,`j`)-th element of `A` (with $0 \le$ `i` $<$ `M` and $0 \le$ `j` $<$ `N`) is given by the expression `(A->data)[j][i]` or by the expression `(A->data)[0][j*M+i]`. The macros below allow a user to efficiently access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer to the `j`-th column of elements can be obtained via the `DENSE_COL` macro. Users should use these macros whenever possible.

9.1.2 Accessor Macros

The following two macros are defined by the DENSE module to provide access to data in the `DenseMat` type:

- `DENSE_ELEM`

  Usage : `DENSE_ELEM(A,i,j) = a_ij;` or `a_ij = DENSE_ELEM(A,i,j);`

  `DENSE_ELEM` references the (`i`,`j`)-th element of the $M \times N$ `DenseMat A`, $0 \le$ `i` $< M$, $0 \le$ `j` $< N$.

- `DENSE_COL`

  Usage : `col_j = DENSE_COL(A,j);`

  `DENSE_COL` references the `j`-th column of the $M \times N$ `DenseMat A`, $0 \le$ `j` $< N$. The type of the expression `DENSE_COL(A,j)` is `realtype *` . After the assignment in the usage above, `col_j` may be treated as an array indexed from 0 to $M - 1$. The (`i`, `j`)-th element of `A` is referenced by `col_j[i]`.

9.1.3 Functions

The following functions for `DenseMat` matrices are available in the DENSE package. For full details, see the header file `sundials_dense.h`.

- `DenseAllocMat`: allocation of a `DenseMat` matrix;
- `DenseAllocPiv`: allocation of a pivot array for use with `DenseGETRF`/`DenseGETRS`;
- `DenseGETRF`: LU factorization with partial pivoting;
- `DenseGETRS`: solution of $Ax = b$ using LU factorization (for square matrices A);
- `DenseZero`: load a matrix with zeros;
- `DenseCopy`: copy one matrix to another;
- `DenseScale`: scale a matrix by a scalar;
- `DenseAddI`: increment a square matrix by the identity matrix;
- `DenseFreeMat`: free memory for a `DenseMat` matrix;
- `DenseFreePiv`: free memory for a pivot array;
- `DensePrint`: print a `DenseMat` matrix to standard output.

9.1.4 Small Dense Matrix Functions

The following functions for small dense matrices are available in the DENSE package:

- `denalloc`

  `denalloc(m,n)` allocates storage for an `m` by `n` dense matrix. It returns a pointer to the newly allocated storage if successful. If the memory request cannot be satisfied, then `denalloc` returns `NULL`. The underlying type of the dense matrix returned is `realtype**`. If we allocate a dense matrix `realtype** a` by `a = denalloc(m,n)`, then `a[j][i]` references the (`i`,`j`)-th element of the matrix `a`, $0 \le$ `i` $<$ `m`, $0 \le$ `j` $< n$, and `a[j]` is a pointer to the first element in the `j`-th column of `a`. The location `a[0]` contains a pointer to `m` $\times$ `n` contiguous locations which contain the elements of `a`.

- `denallocpiv`

  `denallocpiv(n)` allocates an array of `n` integers. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `denGETRF`

  `denGETRF(a,m,n,p)` factors the `m` by `n` dense matrix `a`, using Gaussian elimination with row pivoting. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.

  A successful LU factorization leaves the matrix `a` and the pivot array `p` with the following information:

  1. `p[k]` contains the row number of the pivot element chosen at the beginning of elimination step `k`, `k` $= 0, 1, ...,$`n`-1.
  2. If the unique LU factorization of `a` is given by $Pa = LU$, where P is a permutation matrix, L is an `m` by `n` lower trapezoidal matrix with all diagonal elements equal to 1, and U is an `n` by `n` upper triangular matrix, then the upper triangular part of `a` (including its diagonal) contains U and the strictly lower trapezoidal part of `a` contains the multipliers, $I - L$. If `a` is square, L is a unit lower triangular matrix.

     `denGETRF` returns 0 if successful. Otherwise it encountered a zero diagonal element during the factorization, indicating that the matrix `a` does not have full column rank. In this case it returns the column index (numbered from one) at which it encountered the zero.

- `denGETRS`

  `denGETRS(a,n,p,b)` solves the `n` by `n` linear system $ax = b$. It assumes that `a` (of size `n` $\times$ `n`) has been LU-factored and the pivot array `p` has been set by a successful call to `denGETRF(a,n,n,p)`. The solution x is written into the `b` array.

- `denzero`

  `denzero(a,m,n)` sets all the elements of the `m` by `n` dense matrix `a` to be 0.0;

- `dencopy`

  `dencopy(a,b,m,n)` copies the `m` by `n` dense matrix `a` into the `m` by `n` dense matrix `b`;

- `denscale`

  `denscale(c,a,m,n)` scales every element in the `m` by `n` dense matrix `a` by `c`;

- `denaddI`

  `denaddI(a,n)` increments the `n` by `n` dense matrix `a` by the identity matrix;

- `denfreepiv`

  `denfreepiv(p)` frees the pivot array `p` allocated by `denallocpiv`;

- `denfree`

  `denfree(a)` frees the dense matrix `a` allocated by `denalloc`;

- `denprint`

  `denprint(a,m,n)` prints the `m` by `n` dense matrix `a` to standard output as it would normally appear on paper. It is intended as a debugging tool with small values of `n`. The elements are printed using the `%g` option. A blank line is printed before and after the matrix.

9.2 The BAND module

Relative to the SUNDIALS *srcdir*, the files comprising the BAND generic linear solver are as follows:

- header files (located in *srcdir*`/include/sundials`)
  `sundials_band.h`
  `sundials_types.h` `sundials_math.h` `sundials_config.h`

- source files (located in *srcdir*`/src/sundials`)
  `sundials_band.c` `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are required to use the BAND package by itself (see §2.4 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```

- (optional) use of generic math functions:
  ```
  #define SUNDIALS_USE_GENERIC_MATH 1
  ```

The `sundials_types.h` header file defines of the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the `MIN`, `MAX`, and `ABS` macros and `RAbs` function.

The six files listed above can be extracted from the SUNDIALS *srcdir* and compiled by themselves into a BAND library or into a larger user code.

9.2.1 Type BandMat

The type `BandMat` is the type of a large band matrix A (possibly distributed). It is defined to be a pointer to a structure defined by:

```
typedef struct {
  long int size;
  long int mu, ml, smu;
  realtype **data;
} *BandMat;
```

The fields in the above structure are:

- *size* is the number of columns (which is the same as the number of rows);
- *mu* is the upper half-bandwidth, $0 \le mu \le size-1$;
- *ml* is the lower half-bandwidth, $0 \le ml \le size-1$;
- *smu* is the storage upper half-bandwidth, $mu \le smu \le size-1$. The `BandGBTRF` routine writes the LU factors into the storage for A. The upper triangular factor U, however, may have an upper half-bandwidth as big as min(*size*−1,*mu*+*ml*) because of partial pivoting. The *smu* field holds the upper half-bandwidth allocated for A.
- *data* is a two dimensional array used for component storage. The elements of a band matrix of type `BandMat` are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored.

  If we number rows and columns in the band matrix starting from 0, then

  - *data[0]* is a pointer to (*smu*+*ml*+1)**size* contiguous locations which hold the elements within the band of A
  - *data[j]* is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from *smu*−*mu* (to access the uppermost element within the band in the j-th column) to *smu*+*ml* (to access the lowest element within the band in the j-th column). Indices from 0 to *smu*−*mu*−1 give access to extra storage elements required by `BandGBTRF`.
  - *data[j][i-j+smu]* is the (i, j)-th element, $j-mu \le i \le j+ml$.

The macros below allow a user to access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer into the `j`-th column of elements can be obtained via the `BAND_COL` macro. Users should use these macros whenever possible.

See Figure 9.1 for a diagram of the `BandMat` type.

9.2.2 Accessor Macros

The following three macros are defined by the BAND module to provide access to data in the `BandMat` type:

- `BAND_ELEM`

  Usage : `BAND_ELEM(A,i,j) = a_ij;` or `a_ij = BAND_ELEM(A,i,j);`

  `BAND_ELEM` references the (`i`,`j`)-th element of the $N \times N$ band matrix `A`, where $0 \le$ `i`, `j` $\le N-1$. The location (`i`,`j`) should further satisfy `j-(A->mu)` $\le$ `i` $\le$ `j+(A->ml)`.

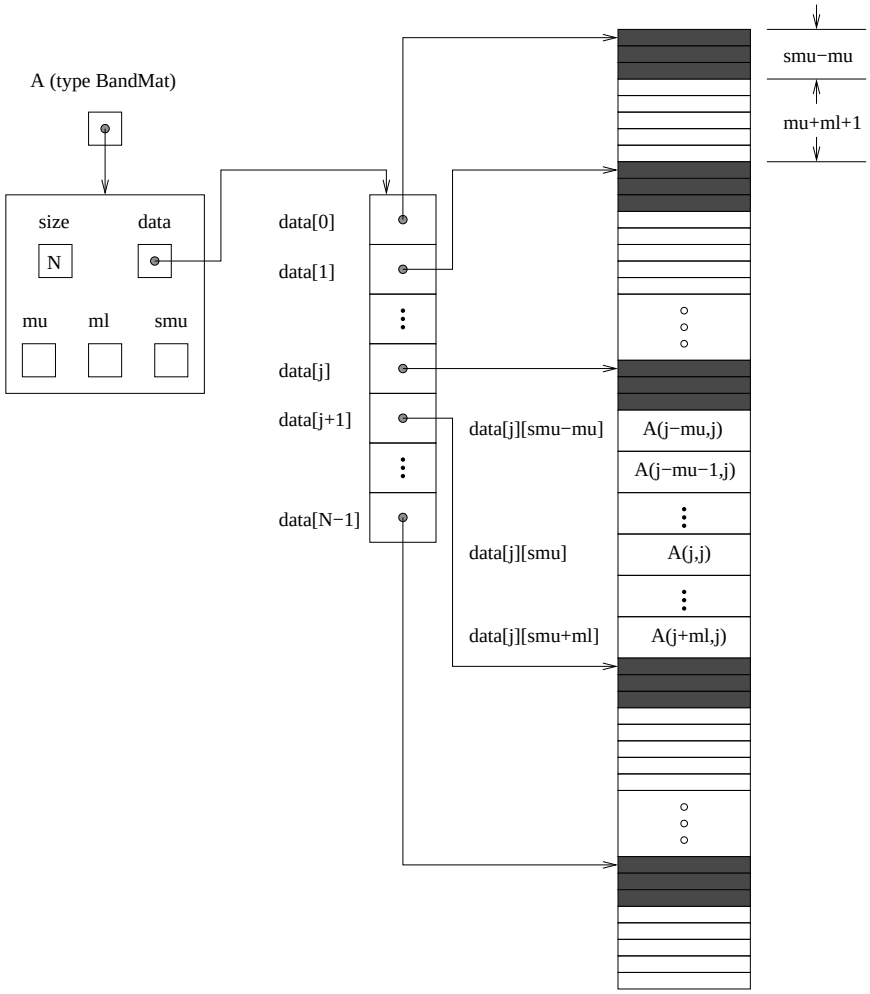

Figure 9.1: Diagram of the storage for a band matrix of type `BandMat`. Here `A` is an $N \times N$ band matrix of type `BandMat` with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to $N-1$ and the (i,j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the `BandGBTRF` and `BandGBTRS` routines.

- BAND_COL

  Usage : col_j = BAND_COL(A,j);

  BAND_COL references the diagonal element of the j-th column of the $N \times N$ band matrix A, $0 \leq$ j $\leq N-1$. The type of the expression BAND_COL(A,j) is realtype *. The pointer returned by the call BAND_COL(A,j) can be treated as an array which is indexed from $-$(A->mu) to (A->ml).

- BAND_COL_ELEM

  Usage : BAND_COL_ELEM(col_j,i,j) = a_ij; or a_ij = BAND_COL_ELEM(col_j,i,j);

  This macro references the (i,j)-th entry of the band matrix A when used in conjunction with BAND_COL to reference the j-th column through col_j. The index (i,j) should satisfy j$-$(A->mu) $\leq$ i $\leq$ j+(A->ml).

9.2.3 Functions

The following functions for BandMat matrices are available in the BAND package. For full details, see the header file sundials_band.h.

- BandAllocMat: allocation of a BandMat matrix;
- BandAllocPiv: allocation of a pivot array for use with BandGBTRF/BandGBTRS;
- BandGBTRF: LU factorization with partial pivoting;
- BandGBTRS: solution of $Ax = b$ using LU factorization;
- BandZero: load a matrix with zeros;
- BandCopy: copy one matrix to another;
- BandScale: scale a matrix by a scalar;
- BandAddI: increment a matrix by the identity matrix;
- BandFreeMat: free memory for a BandMat matrix;
- BandFreePiv: free memory for a pivot array;
- BandPrint: print a BandMat matrix to standard output.

9.3 The SPGMR module

The SPGMR package, in the files sundials_spgmr.h and sundials_spgmr.c, includes an implementation of the scaled preconditioned GMRES method. A separate code module, implemented in sundials_iterative.(h,c), contains auxiliary functions that support SPGMR, as well as the other Krylov solvers in SUNDIALS (SPBCG and SPTFQMR). For full details, including usage instructions, see the header files sundials_spgmr.h and sundials_iterative.h.

Relative to the SUNDIALS *srcdir*, the files comprising the SPGMR generic linear solver are as follows:

- header files (located in *srcdir*/include/sundials)
  sundials_spgmr.h sundials_iterative.h sundials_nvector.h
  sundials_types.h sundials_math.h sundials_config.h
- source files (located in *srcdir*/src/sundials)
  sundials_spgmr.c sundials_iterative.c sundials_nvector.c

Only two of the preprocessing directives in the header file sundials_config.h are required to use the SPGMR package by itself (see §2.4 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```
- (optional) use of generic math functions:
  ```
  #define SUNDIALS_USE_GENERIC_MATH 1
  ```

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the `MAX` and `ABS` macros and `RAbs` and `RSqrt` functions.

The generic NVECTOR files, `sundials_nvector.(h,c)` are needed for the definition of the generic `N_Vector` type and functions. The NVECTOR functions used by the SPGMR module are: `N_VDotProd`, `N_VLinearSum`, `N_VScale`, `N_VProd`, `N_VDiv`, `N_VConst`, `N_VClone`, `N_VCloneVectorArray`, `N_VDestroy`, and `N_VDestroyVectorArray`.

The SPGMR package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The nine files listed above can be extracted from the SUNDIALS *srcdir* and compiled by themselves into an SPGMR library or into a larger user code.

9.3.1 Functions

The following functions are available in the SPGMR package:

- `SpgmrMalloc`: allocation of memory for `SpgmrSolve`;
- `SpgmrSolve`: solution of $Ax = b$ by the SPGMR method;
- `SpgmrFree`: free memory allocated by `SpgmrMalloc`.

The following functions are available in the support package `sundials_iterative.(h,c)`:

- `ModifiedGS`: performs modified Gram-Schmidt procedure;
- `ClassicalGS`: performs classical Gram-Schmidt procedure;
- `QRfact`: performs QR factorization of Hessenberg matrix;
- `QRsol`: solves a least squares problem with a Hessenberg matrix factored by `QRfact`.

9.4 The SPBCG module

The SPBCG package, in the files `sundials_spbcgs.h` and `sundials_spbcgs.c`, includes an implementation of the scaled preconditioned Bi-CGStab method. For full details, including usage instructions, see the file `sundials_spbcgs.h`.

The SPBCG package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The files needed to use the SPBCG module by itself are the same as for the SPGMR module, with `sundials_spbcgs.(h,c)` replacing `sundials_spgmr.(h,c)`.

9.4.1 Functions

The following functions are available in the SPBCG package:

- `SpbcgMalloc`: allocation of memory for `SpbcgSolve`;
- `SpbcgSolve`: solution of $Ax = b$ by the SPBCG method;
- `SpbcgFree`: free memory allocated by `SpbcgMalloc`.

9.5 The SPTFQMR module

The SPTFQMR package, in the files `sundials_sptfqmr.h` and `sundials_sptfqmr.c`, includes an implementation of the scaled preconditioned TFQMR method. For full details, including usage instructions, see the file `sundials_sptfqmr.h`.

The SPTFQMR package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The files needed to use the SPTFQMR module by itself are the same as for the SPGMR module, with `sundials_sptfqmr.(h,c)` replacing `sundials_spgmr.(h,c)`.

9.5.1 Functions

The following functions are available in the SPTFQMR package:

- `SptfqmrMalloc`: allocation of memory for `SptfqmrSolve`;
- `SptfqmrSolve`: solution of $Ax = b$ by the SPTFQMR method;
- `SptfqmrFree`: free memory allocated by `SptfqmrMalloc`.

Chapter 10

IDA Constants

Below we list all input and output constants used by the main solver and linear solver modules, together with their numerical values and a short description of their meaning.

10.1 IDA input constants

IDA **main solver module**		
IDA_SS	1	Scalar relative tolerance, scalar absolute tolerance.
IDA_SV	2	Scalar relative tolerance, vector absolute tolerance.
IDA_NORMAL	1	Solver returns at specified output time.
IDA_ONE_STEP	2	Solver returns after each successful step.
IDA_NORMAL_TSTOP	3	Solver returns at specified output time, but does not proceed past the specified stopping time.
IDA_ONE_STEP_TSTOP	4	Solver returns after each successful step, but does not proceed past the specified stopping time.
IDA_YA_YDP_INIT	1	Compute y_a and y'_d, given y_d.
IDA_Y_INIT	2	Compute y, given y'.

Iterative linear solver module		
PREC_NONE	0	No preconditioning
PREC_LEFT	1	Preconditioning on the left.
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

10.2 IDA output constants

IDA **main solver module**		
IDA_SUCCESS	0	Successful function return.
IDA_TSTOP_RETURN	1	IDASolve succeeded by reaching the specified stopping point.
IDA_ROOT_RETURN	2	IDASolve succeeded and found one or more roots.
IDA_MEM_NULL	-1	The ida_mem argument was NULL.
IDA_ILL_INPUT	-2	One of the function inputs is illegal.
IDA_NO_MALLOC	-3	The IDA memory was not allocated by a call to IDAMalloc.
IDA_TOO_MUCH_WORK	-4	The solver took mxstep internal steps but could not reach tout.

IDA_TOO_MUCH_ACC	-5	The solver could not satisfy the accuracy demanded by the user for some internal step.
IDA_ERR_FAIL	-6	Error test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_CONV_FAIL	-7	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_LINIT_FAIL	-8	The linear solver's initialization function failed.
IDA_LSETUP_FAIL	-9	The linear solver's setup function failed in an unrecoverable manner.
IDA_LSOLVE_FAIL	-10	The linear solver's solve function failed in an unrecoverable manner.
IDA_RES_FAIL	-11	The user-provided residual function failed in an unrecoverable manner.
IDA_CONSTR_FAIL	-12	The inequality constraints were violated and the solver was unable to recover.
IDA_REP_RES_FAIL	-13	The user-provided residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_MEM_FAIL	-14	A memory allocation failed.
IDA_BAD_T	-15	The time t s outside the last step taken.
IDA_BAD_EWT	-16	Zero value of some error weight component.
IDA_FIRST_RES_FAIL	-17	The user-provided residual function failed recoverably on the first call.
IDA_LINESEARCH_FAIL	-18	The line search failed.
IDA_NO_RECOVERY	-19	The residual function, linear solver setup function, or linear solver solve function had a recoverable failure, but IDACalcIC could not recover.
IDA_RTFUNC_FAIL	-20	The rootfinding function failed in an unrecoverable manner.

IDADENSE linear solver module

IDADENSE_SUCCESS	0	Successful function return.
IDADENSE_MEM_NULL	-1	The ida_mem argument was NULL.
IDADENSE_LMEM_NULL	-2	The IDADENSE linear solver has not been initialized.
IDADENSE_ILL_INPUT	-3	The IDADENSE solver is not compatible with the current NVECTOR module.
IDADENSE_MEM_FAIL	-4	A memory allocation request failed.
IDADENSE_JACFUNC_UNRECVR	-5	The Jacobian function failed in an unrecoverable manner.
IDADENSE_JACFUNC_RECVR	-6	The Jacobian function had a recoverable error.

IDABAND linear solver module

IDABAND_SUCCESS	0	Successful function return.
IDABAND_MEM_NULL	-1	The ida_mem argument was NULL.
IDABAND_LMEM_NULL	-2	The IDABAND linear solver has not been initialized.
IDABAND_ILL_INPUT	-3	The IDABAND solver is not compatible with the current NVECTOR module.
IDABAND_MEM_FAIL	-4	A memory allocation request failed.
IDABAND_JACFUNC_UNRECVR	-5	The Jacobian function failed in an unrecoverable manner.
IDABAND_JACFUNC_RECVR	-6	The Jacobian function had a recoverable error.

IDASPILS linear solver modules		
IDASPILS_SUCCESS	0	Successful function return.
IDASPILS_MEM_NULL	-1	The ida_mem argument was NULL.
IDASPILS_LMEM_NULL	-2	The linear solver has not been initialized.
IDASPILS_ILL_INPUT	-3	The solver is not compatible with the current NVECTOR module.
IDASPILS_MEM_FAIL	-4	A memory allocation request failed.

SPGMR generic linear solver module		
SPGMR_SUCCESS	0	Converged.
SPGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPGMR_CONV_FAIL	2	Failure to converge.
SPGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPGMR_ATIMES_FAIL_REC	5	The Jacobian-times-vector function failed recoverably.
SPGMR_PSET_FAIL_REC	6	The preconditioner setup function failed recoverably.
SPGMR_MEM_NULL	-1	The SPGMR memory is NULL
SPGMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPGMR_QRSOL_FAIL	-5	The matrix R was found to be singular during the QR solve phase.
SPGMR_PSET_FAIL_UNREC	-6	The preconditioner setup function failed unrecoverably.

SPBCG generic linear solver module		
SPBCG_SUCCESS	0	Converged.
SPBCG_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPBCG_CONV_FAIL	2	Failure to converge.
SPBCG_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPBCG_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPBCG_PSET_FAIL_REC	5	The preconditioner setup function failed recoverably.
SPBCG_MEM_NULL	-1	The SPBCG memory is NULL
SPBCG_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPBCG_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPBCG_PSET_FAIL_UNREC	-4	The preconditioner setup function failed unrecoverably.

SPTFQMR generic linear solver module		
SPTFQMR_SUCCESS	0	Converged.
SPTFQMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPTFQMR_CONV_FAIL	2	Failure to converge.
SPTFQMR_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPTFQMR_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPTFQMR_PSET_FAIL_REC	5	The preconditioner setup function failed recoverably.

SPTFQMR_MEM_NULL	-1	The SPTFQMR memory is NULL
SPTFQMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed.
SPTFQMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPTFQMR_PSET_FAIL_UNREC	-4	The preconditioner setup function failed unrecoverably.

IDABBDPRE **preconditioner module**

IDABBDPRE_SUCCESS	0	Successful function return.
IDABBDPRE_PDATA_NULL	-11	The preconditioner module has not been initialized.
IDABBDPRE_FUNC_UNRECVR	-12	A user supplied function failed unrecoverably.

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