ADIFOR 2.0 User’s Guide

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ADIFOR 2.0 Users’ Guide
(Revision D)

by

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Chapter 1

Miscellany

1.1 Supported Systems

ADIFOR 2.0 currently runs on SPARC’s running SunOS 4.1 or SunOS 5.x (Solaris 2.x), IBM
RS/6000’s running AIX 3.2.5 or 4.1.1, SGI workstations running IRIX Release 6.2, HP workstations
running HP-UX 9.x, and x86-class personal computers running Linux, Windows 95 or Windows NT.
ADIFOR 2.0 will be ported to additional computing platforms if we find sufficient interest and have
access to that platform.

1.2 How to Get ADIFOR 2.0

To retrieve the ADIFOR 2.0 automatic differentiation software for educational and non-profit re-
search use, and for commercial evaluation, visit either of the ADIFOR group World Wide Web
These pages describe how to request access to ADIFOR 2.0 and how to download the software. The
pages also contain links to publications related to ADIFOR, including many of the papers referenced
in this user’s guide, as well as the most recent version of this user’s guide.

1.3 Legal Notices

Copyright on the ADIFOR Preprocessor is held by Rice University. Copyright on the ADIntrinsics
system and the SparsLinC libraries is held by the University of Chicago.

ADIFOR 2.0 was prepared as an account of work sponsored by an agency of the United States
Government, Rice University, and the University of Chicago. NEITHER THE AUTHOR(S), THE
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NESS OF ANY INFORMATION OR PROCESS DISCLOSED, OR REPRESENTS THAT ITS
USE WOULD NOT INFRINGE PRIVATELY OWNED RIGHTS.

If ADIFOR 2.0 has been installed at your site in the usual manner, then a copy of the public
license for ADIFOR 2.0 can be found in $AD_HOME/LICENSE. The license is also available at both of
the World Wide Web sites listed in Section 1.2.
Any entity desiring permission to incorporate this software or a work based on the software into commercial products or otherwise use it for commercial purposes should contact:

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Chapter 2

Some Preliminaries

Automatic differentiation is a technique for computing the derivatives of functions described by computer programs. See [18, 24] for an introduction to automatic differentiation. ADIFOR implements automatic differentiation by transforming a collection of FORTRAN 77 subroutines that compute a function $f$ into new FORTRAN 77 subroutines that compute the derivatives of the outputs of $f$ with respect to a specified set of inputs of $f$. This paper describes step by step how to use version 2.0 (Revision D) of the ADIFOR system to generate derivative code. Familiarity with UNIX\(^1\) and FORTRAN 77 is assumed.

We strongly suggest that you, before reading this manual, have a look at the overview papers of ADIFOR 2.0 [7] and ADIFOR 1.0 [6]. They provide an overview of the philosophy of ADIFOR, references to successful applications of ADIFOR, and a perspective of how automatic differentiation relates to other approaches for computing derivatives.

The ADIFOR 2.0 system consists of the ADIFOR Preprocessor, the ADIntrinsics template expander and library, and the SparsLinC library. The `adifor2.1` command invokes both the preprocessor and the ADIntrinsics template expander. Figure 2.1 presents a block diagram of the ADIFOR 2.0 process, which consists of three key steps:

1. Apply the ADIFOR Preprocessor to your FORTRAN 77 program to produce augmented code for the computation of derivatives. The preprocessor invokes the ADIntrinsics template expander directly. We refer to the machine on which you execute the preprocessor as ADIFORHOST.

2. Construct a derivative driver code that invokes the generated derivative code and makes use of the computed derivatives.

3. Compile the generated derivative code and your derivative driver code, and link these with the derivative support packages, i.e., the ADIntrinsics exception handling package (see Appendix B), and (optionally) the SparsLinC sparse derivative package (see Appendix C). We refer to the machine on which you compile and link your derivative driver code and the ADIFOR 2.0 support packages as EXECHOST. Notice that ADIFORHOST and EXECHOST may be different, for example, ADIFORHOST may be a SPARC workstation, and EXECHOST an RS6000.

The first step of this process can be performed on SPARC's running SunOS 4.1 or SunOS 5.x (Solaris 2.x), IBM RS/6000's running AIX 3.2.5 or 4.1.1, SGI workstations running IRIX Release 6.2, HP workstations running HP-UX 9.x, and x86-class personal computers running Linux, Windows 95

\(^1\)UNIX is a trademark of AT&T.
Figure 2.1. Block Diagram of the ADIFOR Process
or Windows NT. ADIFORHOST is, therefore, currently limited to be a SPARC, an IBM RS/6000
or, an SGI workstation, an HP workstation, or an x86-class personal computer. We currently
provide the necessary libraries for the second step precompiled for each of the machines listed above.
Source code for the libraries is also provided in case you need to compile them to execute on other
architectures. A "C" compiler is required to compile the SparsLinC library. It should, therefore, be
possible to use any machine as EXEHOST.

2.1 Installation

All of these files in the ADIFOR 2.0 distribution can be retrieved from the World Wide Web sites
documented in Section 1.2 of this guide. The distribution consists of the following files:

- **Readme.txt** provides late-breaking news about the ADIFOR 2.0 distribution, including an-
nouncements of the availability of precompiled versions of the ADIFOR 2.0 executables and
libraries for new architectures.
- **InstallGuideUnix.txt** and **InstallGuideWindows.txt** list the steps required to install AD-
IFOR 2.0 on your system.
- **ad2.0D-XXXX.tar.gz** is a gzip-compressed UNIX tar format file. **XXXX** is one of SunOS-4.x,
  SunOS-5.x, AIX, IRIX, HpuX, or Linux86.
- **ad2D.exe** is a self-extracting installer for Windows 95 and Windows NT.

The files **ad2.0D-XXXX.tar.gz** and **ad2D.exe** unpack into two directories named **ADIFOR2.0D**
and **ADIFOR2.0D.lib**.

Directory **ADIFOR2.0D** contains:

- **bin**: Contains **Adifor2.1**, the ADIFOR Preprocessor, and **purse**, the ADIntrinsics template
  expander. The template expander is responsible for expanding generic exception-handling
  macros introduced by ADIFOR 2.0 into the appropriate FORTRAN 77 code. The **purse**
  executable is a **perl** script.\(^2\)
- **templates**: Contains the definition of the exception handling macros used by **purse**.
- **docs**: Contains postscript versions of relevant working notes and papers, including this manual.
- **examples**: Contains examples of programs processed with ADIFOR 2.0.
- **man**: Contains the man page for ADIFOR 2.0.
- **perl.lib**: Contains the **perl** libraries required by **purse**.

Directory **ADIFOR2.0D.lib** contains:

- **src**: Contains the source for the ADIntrinsics and SparsLinC libraries.
- **lib**: Contains the precompiled versions of the ADIntrinsics and SparsLinC libraries.
- **bin**: Contains several auxiliary binaries for use in building the libraries.

\(^2\) We have provided executables for **perl** version 5 in case it is unavailable on your system. To avoid conflicts with
any version of **perl** you have installed on your system, we have named our copies of **perl** to be **perl-$ADJS**. The
**purse** executable invokes the copy of **perl** that we have provided using this name.
<table>
<thead>
<tr>
<th>Machine/OS</th>
<th>compressed tar file</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPARC/SunOS 4.1.x</td>
<td>ad2.0D-SunOS-4.x.tar.gz</td>
</tr>
<tr>
<td>SPARC/SunOS 5.x (Solaris 2.x)</td>
<td>ad2.0D-SunOS-5.x.tar.gz</td>
</tr>
<tr>
<td>RS/6000/AIX 3.2.5 or 4.1.1</td>
<td>ad2.0D-AIX.tar.gz</td>
</tr>
<tr>
<td>SGI/IRIX 6.2</td>
<td>ad2.0D-IRIX.tar.gz</td>
</tr>
<tr>
<td>HP/HPUX 9.x</td>
<td>ad2.0D-Hpux.tar.gz</td>
</tr>
<tr>
<td>x86/Linux</td>
<td>ad2.0D-Linux86.tar.gz</td>
</tr>
</tbody>
</table>

Table 2.1. Machine to Archive Mapping

<table>
<thead>
<tr>
<th>Machine/OS</th>
<th>AD_OS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPARC/SunOS 4.1.x</td>
<td>SunOS-4.x</td>
</tr>
<tr>
<td>SPARC/SunOS 5.x (Solaris 2.x)</td>
<td>SunOS-5.x</td>
</tr>
<tr>
<td>RS/6000/AIX</td>
<td>AIX</td>
</tr>
<tr>
<td>SGI/IRIX</td>
<td>IRIX</td>
</tr>
<tr>
<td>HP/HPUX 9.x</td>
<td>Hpux</td>
</tr>
<tr>
<td>x86/Linux</td>
<td>Linux6</td>
</tr>
<tr>
<td>Cray T3E</td>
<td>Unicos</td>
</tr>
</tbody>
</table>

Table 2.2. Machine to AD_OS Mapping

Each UNIX tar file `ad2.0D-XXXX.tar.gz` contains an executable version of the ADIFOR Preprocessor for the operating system defined by `XXXX`. Similarly, `ad20D.exe` contains the Windows 95/NT executable for the preprocessor. Each of these distribution files however, contain precompiled versions of the ADIntrinsics and SparsoLinC packages for all of the currently supported machines.

If you intend to run ADIFOR 2.0 on multiple kinds of machines then you will need to download and unpack several of the `ad2.0D-XXXX.tar.gz` or `ad20D.exe` files — one for each of the kinds of machine you intend to use as ADIFORHOST and EXECHOST. You may want to delete the unnecessary libraries that you get on ADIFORHOST after you unpack the tar files.

We now describe the installation and configuration procedure for ADIFOR 2.0 under Unix and Windows 95/NT.

### 2.1.1 Unix Installation and Configuration

To install ADIFOR 2.0 on one of the supported UNIX machines, you should first download the appropriate `gzip`-compressed tar file. Table 2.1 provides the names for these files. Once you have downloaded the file, you should move it into the directory in which you wish to place the `ADIFOR2.0D` and `ADIFOR2.0D.lib` directories, and then “un-gzip” and “untar” the file using the following commands:

```
% gunzip ad2.0D-XXXX.tar.gz
% tar xf ad2.0D-XXXX.tar
```

or

```
% gun tar zxf ad2.0D-XXXX.tar.gz
```

where `XXXX` is one of SunOS-4.x, SunOS-5.x, AIX, IRIX, Hpux, or Linux86.\(^3\)

\(^3\)If necessary, you should download a copy of `gunzip` or `gun tar` from ftp://prep.ai.mit.edu/pub/gnu/.
To configure ADIFOR 2.0, set the environment variable AD_HOME to be the path to the directory ADIFOR2.0.D, AD_LIB to be the path to the directory ADIFOR2.0.D.lib, and the variable AD_OS as indicated in Table 2.2.

```
setenv AD_HOME /usr/local/ADIFOR2.0
setenv AD_LIB /usr/local/ADIFOR2.0.lib
setenv PATH $AD_HOME/bin:$PATH
setenv MANPATH $AD_HOME/man:$MANPATH
setenv AD_OS SunOS-4.x
```

Figure 2.2. Portion of .cshrc File

The directories "$AD_HOME/bin" and "$AD_HOME/man" should be added to your execution and manual paths, respectively. (The notation $X represents the value of the environment variable X.) If you use csh or a variant thereof, we suggest modifying your "cshrc" file to define AD_HOME and to modify your execution and manual paths. Figure 2.2 shows a fragment of a "cshrc" file that has been modified assuming that ADIFORHOST and EXECHOSt are the same machine, and that the ADIFOR2.OD and ADIFOR2.OD.lib directories have been installed in /usr/local on a SPARC running SunOS 4.1.3. If you are using a shell other than csh, then use the appropriate commands to modify your environment variables.

The rest of this manual assumes that you have set AD_HOME and AD_LIB and modified your execution path and manual path as just described. It is also assumed that ADIFORHOST and EXECHOSt are the same machine.

To link the ADIntrinsics package into an executable under UNIX4, you should use a command of the form (assuming that f77 is the Fortran 77 compiler)

```
f77 -o adnewton adnewton.o g_func.o dlang.e dgesv.o ...
$AD_LIB/lib/ReqADIntrinsics-$AD_OS.o
$AD_LIB/lib/libADIntrinsics-$AD_OS.a
```

or, equivalently,

```
f77 -o adnewton adnewton.o g_func.o dlang.e dgesv.o ...
$AD_LIB/lib/ReqADIntrinsics-$AD_OS.o
-L $AD_LIB/lib -LADIntrinsics-$AD_OS
```

Similarly, to link the SparsLinC package into an executable, use

```
f77 -o adnewton adnewton.o g_func.o dlang.e dgesv.o ...
$AD_LIB/lib/libSparsLinC-$AD_OS.a
```

or

```
f77 -o adnewton adnewton.o g_func.o dlang.e dgesv.o ...
-L $AD_LIB/lib -LSparsLinC-$AD_OS
```

---

4Under IRIX on an SGI workstation, the libraries that are identified with the IRIX suffix have been compiled with the -m32 compiler flags. If you need to use -o32 or -64 compiler options, then use the libraries with suffix IRIX-o32 or IRIX-64, respectively.
2.1.2 Windows 95/NT Installation and Configuration

To install ADIFOR 2.0 on a x86-class PC running Windows 95/NT, you should download the file ad20d.exe. Executing this “self-extracting installer” will allow you to unpack all of the necessary files into a directory that you select. Do not extract the files contained in ad20d.exe into a directory whose pathname contains space characters. For example, do not attempt to install ADIFOR 2.0 into C:\Program Files\Adifor.

To configure ADIFOR 2.0 under Windows-95/NT, we suggest that you modify your autoexec.bat file to include the following commands (assuming that you have installed ADIFOR into directory C:\Adifor):

```
SET PATH=C:\Adifor\Adifor2.0D\bin;%PATH%;
SET AD_HOME=C:\Adifor\Adifor2.0D
SET AD_LIB=C:\Adifor\Adifor2.0D.lib
```

The Windows 95/NT version of ADIFOR 2.0 also contains the file examples.zip in the Adifor Adifor2.0D directory. You should be able to unpack these under Windows 95/NT using any modern version of “zip” on the PC.

To link the ADIntrinsics package into an executable under Windows 95/NT, you should use a command of the form:

```
link *.obj %AD_LIB%\lib\ReqADIntrinsics.obj \
     %AD_LIB%\lib\ADIntrinsics.lib /out:adnewton.exe
```

Similarly, to link the SpursLinC package into an executable, use

```
link *.obj %AD_LIB%\lib\SparsLinC.lib /out:adnewton.exe
```

2.2 Building the Libraries

It is sometimes necessary to build the ADIntrinsics and SpursLinC libraries from the source code provided. The source code for the ADIntrinsics and SpursLinC libraries are stored in subdirectories ADIntrinsics and SpursLinC of directory ADIFOR2.0D.lib/src.

The UNIX csh script Compile.Intrinsics in the ADIntrinsics directory and the csh script Compile.SparsLinC in the SpursLinC directory are used to build the libraries. To use these scripts, you will need to define a set of environment variables described in the comments at the top of each script, and then execute the script. These scripts build the libraries in the ADIntrinsics and SpursLinC subdirectories, so do not forget to copy them to the ADLIB directory or modify the ADLIB variable accordingly.

The Windows batch command files CompileADIntrinsics.bat and CompileSparsLinC.bat are used to build the libraries under Windows 95/NT. In contrast to the Unix scripts, these scripts copy the compiled libraries into the ADLIB directory.

2.3 How the ADIFOR Preprocessor Transforms a Program

In this section, we describe the mechanism used by the ADIFOR Preprocessor to transform your FORTRAN 77 code into code that computes derivatives of dependent variables with respect to independent variables. The mechanism has three key subtasks: code canonicalization, variable nomination, and code generation. Understanding these three tasks will help you better understand the derivative code that is generated. We briefly describe these subtasks in the next sections.
2.3.1 Code Canonicalization

In the code canonicalization phase, the FORTRAN 77 code is rewritten into a standard form. For example, expressions appearing as arguments to function or subroutine calls and function calls appearing within conditional tests are hoisted into assignments to new temporary variables. Statement functions are expanded into in-line code. This phase also breaks up long right-hand sides of assignment statements into smaller pieces, and rewrites them such that all variables appearing on the right-hand side of an assignment statement are of the same type. The latter transformation is needed for the code to be able to link in the SparsLinC library (see Appendix C).

2.3.2 Variable Nomination

The ADIFOR Preprocessor must decide which variables need to have “directional gradient objects” or “gradient objects” associated with them. The preprocessor associates a gradient object with every variable whose value may depend on the value of a variable considered “independent” with respect to differentiation, and whose value impacts a variable considered “dependent” with respect to differentiation. Such a variable is called active. Variables that do not require derivative information are called passive.

The ADIFOR Preprocessor employs interprocedural analysis techniques to determine which variables in your code are active. First, it derives a “local interaction graph” for each subroutine. This is a bipartite graph where nodes representing input parameters or variables in common blocks are connected with nodes representing output parameters or variables in common blocks whose values they influence.

Next, an interprocedural analysis is performed, which determines, in essence, all possible program paths through which an independent variable can affect a dependent one and identifies intermediate variables that are involved along such a path. This analysis involves computing a transitive closure of the whole program graph composed from the local interaction graphs. In the presence of common blocks, equivalences, and arbitrary control structures, this is a nontrivial and computationally intensive process.

2.3.3 Code Generation

After active variables have been nominated, derivative code is generated for each assignment statement containing an active variable, and gradient objects are allocated. For assignment statements containing a FORTRAN 77 intrinsic, a template is generated that will later be instantiated by the ADIntrinsics system.

2.4 Functionality of ADIFOR 2.0-Generated Code

Consider a function \texttt{func} with an \texttt{n}-vector \texttt{x} as independent and an \texttt{m}-vector \texttt{y} as dependent variables. That is, we have

```fortran
subroutine func(n,x,m,y)
    integer n, m
    real x(n), y(m)
    ...
    end
```
The ADIFOR Preprocessor inserts a gradient object $g_x$ for $x$ and $g_y$ for $y$ (as well as gradient objects for all other active variables in func) and, in its default configuration, replaces each assignment statement in func involving an active variable with a few assignment statements and a vector loop from 1 to $g_p$. The interface of the routine generated from func is

```fortran
subroutine g_func(g_p, n, x, ldg_x, y, ldg_y)
  integer n, m, g_p
  real x(n), y(m), g_x(ldg_x, n), g_y(ldg_y, m)
  ...
end
```

So, for example, $g_x(:,1)$ is the gradient object corresponding to $x(1)$. While somewhat inconvenient, the fact that the gradient dimension is the first dimension in the gradient objects cannot be avoided if we want to be able to deal with assumed-size arrays (e.g., declared as real $x(\star)$).

We now illustrate the flexibility inherent in the ADIFOR 2.0-generated code. First, recall the definition of the Jacobian of func,

$$
J = \frac{d}{d \mathbf{x}} \mathbf{y} = 
\begin{pmatrix}
\frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\
\vdots & & \vdots \\
\frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n}
\end{pmatrix}
\in \mathbb{R}^{m \times n}.
$$

Second, let $S = g_x^T$. We refer to $S$ as the “seed matrix.” The ADIFOR-generated code computes

$$
g_y = (\frac{\partial y}{\partial x} \times g_x)^T = (J \ast S)^T,
$$

where the number of columns $p$ of $S$ corresponds to the FORTRAN 77 variable $g_p$ in the generated code. Since most of the work of the derivative code is performed in the gradient loops (which range from 1 to $g_p$), the size of $p$ has a direct impact on the runtime and storage requirements for running the derivative code.

Properly initializing $S$, we can then obtain:

**Full Jacobian:** Choosing $S$ as the $n \times n$ identity matrix, we compute the transpose of the full Jacobian $J$. The complexity of the resulting derivative code is $O(n)$ times that of the original function.

**Jacobian-Vector Product:** Choosing $S = d \in \mathbb{R}^n$, we compute the transpose of the Jacobian-vector product $Jd$ in a time that is a small multiple (typically 2-3) of the function evaluation time. Since

$$
Jd = \lim_{h \to 0} \frac{\text{func}(x + hd) - \text{func}(x)}{h},
$$

this interface allows us to compute directional derivatives along arbitrary directions.

**Selecting Derivatives:** Choosing $S = [\epsilon_5, \ldots, \epsilon_{10}, \epsilon_{13}]$, where $\epsilon_i$ is the $i$th canonical unit vector, i.e., an $n$-vector of all zeros except for an entry of 1 in the $i$th position, we compute the transpose of the 5th through 10th, and 13th columns of $J$.

See Appendix A for extensive information on seed matrix initialization. In particular, it explains how to deal with several dependent and independent variables and how to exploit sparsity in the Jacobian $J$. 

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2.5 A Quick Example

We demonstrate the use of ADIFOR 2.0, using its default configurations, with the very simple program shown in Figures 2.3 and 2.4. Procedure \texttt{squareroott} assigns the square root of the value of variable \texttt{x} to variable \texttt{y}. We now show, with only limited explanation, the sequence of steps required to construct a procedure that computes the derivative of \texttt{squareroott} at a user-specified value of \texttt{x}. A more detailed description of the ADIFOR 2.0 process and of the various options available in the ADIFOR Preprocessor is presented in Chapter 4.

1. Construct a composition \texttt{simple.cmp} that lists the names of all of the FORTRAN 77 source files that constitute the example program. Figure 2.5 shows the composition we construct.

2. Construct a script file \texttt{simple.adf} that tells the ADIFOR Preprocessor to differentiate the procedure named \texttt{squareroott} with the independent variable \texttt{x} and the dependent variable \texttt{y}, i.e., to generate code to compute the derivative \( \frac{dy}{dx} \), where \texttt{y} is computed from \texttt{x} by procedure \texttt{squareroott}. The script file is shown in Figure 2.6.

3. Create, in \texttt{g.squareroott.f} file in the \texttt{output_files} subdirectory, the procedure \texttt{g.squareroott}, as shown in Figure 2.7, by executing the command

\begin{verbatim}
Adifor2.1 AD_SCRIPT=simple.adf.
\end{verbatim}

Note that an exception handler (\texttt{ehufSV}) is invoked when \texttt{sqrt} is invoked with a zero argument, as the derivative of \( \sqrt{y} \) is undefined. The ADIFOR Preprocessor also creates a file called \texttt{main.f} and \texttt{squareroott.f}.

```plaintext
Figure 2.3. A Very Simple Program (\texttt{main.f})
```

```plaintext
subroutine squareroott(x, y)
real x, y
y = sqrt(x)
end
```

```plaintext
Figure 2.4. A Very Simple Subroutine (\texttt{squareroott.f})
```

```plaintext
Figure 2.5. Script File (\texttt{simple.cmp}) for Simple Example
```
\begin{verbatim}
AD_TOP    = squareroot
AD_PMAX   = 1
AD_IVARS  = x
AD_DVARS  = y
AD_PROG   = simple.cmp

subroutine g_squareroot(g_p_, x, g_x, ldg_x, y, g_y, ldg_y)
real x, y
integer g_pmax_
parameter (g_pmax_ = 1)
integer g_i_, g_p_, ldg_y, ldg_x
real r1_p, r2_v, g_y(ldg_y), g_x(ldg_x)
integer g_ehfid
data g_ehfid /0/
if (g_p_ .gt. g_pmax_) then
  print *, 'Parameter g_p_ is greater than g_pmax_'
  stop
endif
r2_v = sqrt(x)
if ( x .gt. 0.0e0 ) then
  r1_p = 1.0e0 / (2.0e0 * r2_v)
else
  call ehfSV (9, x, r2_v, r1_p, 'g_squareroot.f', 37)
endif
do g_i_ = 1, g_p_
  g_y(g_i_) = r1_p * g_x(g_i_)
endo
y = r2_v
C--------
end
\end{verbatim}

Figure 2.6. Script File (simple.adf) for Simple Example

Figure 2.7. Derivative Code (g_squareroot.f)
program driver
real x, y
real g_x(1), g_y(1)
read *, x
g_x(1) = 1.0
call g_squareroot(1, x, g_x, 1, y, g_y, 1)
call ehrpt
print *, y
print *, g_y(1)
end

Figure 2.8. Derivative Code Driver (driver.f) for Simple Example

f77 -c driver.f
f77 -c output_files/g_squareroot.f
f77 -o driver driver.o g_squareroot.o
   $AD_LIB/lib/ReqADIntrinsics-$AD_OS.o
   $AD_LIB/lib/ADIntrinsics-$AD_OS.a

Figure 2.9. Commands to Compile and Link Derivative Code Executable

g_squareroot.A in the output_files subdirectory, which differs from g_squareroot.f only
inasmuch as the code for the intrinsics exception handling has not been instantiated yet.
Usually, there is no need for the user to look at the .A files. Appendix B describes this issue
in more detail.

4. Create the derivative code driver driver.f as shown in Figure 2.8. The driver invokes
g_squareroot with a user-specified value of x to compute the value of y and \[\frac{dy}{dx}\]. The call
to the error handler reporting routine ehrpt produces a summary report on FORTRAN 77
intrinsics that were invoked at points of non-differentiability (see Appendix B for details).

5. Compile and link driver.f, g_squareroot.f and the ADIntrinsics exception handling libraries
using the commands shown in Figure 2.9 to build the desired derivative computing executable⁵

2.6 A Roadmap

The rest of this manual is organized as follows:

Chapter 3 describes how to set up the inputs to the ADIFOR Preprocessor to enable it to generate
derivative code. The input to the preprocessor takes the form of option bindings that are
specified on the command line or in startup files, and compositions, lists of FORTRAN 77 files
that constitute the program that contains the function to be differentiated.

⁵If you should incur problems linking on a SPARC platform, you may not have the latest version of the Sun Fortran
compiler installed. You should recompile the libraries from the source we provide as described in section 2.2.
Chapter 4 is devoted to a step-by-step description of how to process a code by using the ADIFOR Preprocessor and an explanation of how ADIFOR 2.0-generated code should be incorporated into a program.

Chapter 5 documents the known deficiencies in the ADIFOR Preprocessor’s support for FORTRAN 77. For each deficiency, a workaround is presented.

Chapter 6 explains how to use ADIFOR 2.0 in cases where the “function to be differentiated” does not have the form expected by the ADIFOR Preprocessor.

Chapter 7 covers some of the pitfalls associated with automatic differentiation of FORTRAN 77 programs.

Chapter 8 provides a list of problems that users of ADIFOR 2.0 may encounter.

Chapter 9 defines all of the options to the ADIFOR Preprocessor and presents their default values.

Appendix A describes seed matrix initialization, a powerful concept that provides users of ADIFOR 2.0 significant control over the computation performed by the generated derivative code, and allows one to compute arbitrary directional derivatives.

Appendix B describes the ADIntrinsics template expander and library. ADIntrinsics provides user-customizable handling of exceptions within ADIFOR 2.0.

Appendix C describes the SparsLinC library, which provides support for sparse derivative computations within ADIFOR 2.0.
Chapter 3

Specifying Input for the ADIFOR Preprocessor

In order to apply the ADIFOR Preprocessor to a set of FORTRAN 77 procedures to generate derivative code, it is necessary to tell it several key pieces of information:

1. The names of the files containing the FORTRAN 77 source code to be processed. The names of the procedures are provided to the ADIFOR Preprocessor in a file referred to as a composition. The preprocessor must be told the name of the file containing the composition.

2. The name of the “top-level routine,” that routine whose invocation causes the function to be evaluated. The ADIFOR Preprocessor determines the names of all of the routines that may be transitively invoked by the top routine by examining the source code.

3. The names of the independent and dependent variables. The ADIFOR 2.0-generated code computes the derivatives of the dependent variables with respect to the independent ones.

4. Values of numerous other options to the ADIFOR Preprocessor that control how vector operations in the ADIFOR-generated code are implemented, what level of exception reporting for nondifferentiable FORTRAN 77 intrinsics is performed, and to what extent the code should be customized for particular execution environments.

The names of the composition file, the top routine, and the independent and dependent variables, and values for the various options, are provided to the ADIFOR Preprocessor in the form of bindings, as described in the next section. Section 3.2 describes the format of compositions. Section 3.3 describes source files that are acceptable for processing with the preprocessor and describes some common deviations from the FORTRAN 77 standard that cause problems.

3.1 Option Processing in the ADIFOR Preprocessor

This section describes the ADIFOR Preprocessor’s option-processing mechanism. Information is provided to the preprocessor as bindings. Bindings have the form

\[
\text{OPTION} = \text{VALUE},
\]

or

\[
\text{OPTION} = \text{VALUE1, \ldots, VALUEN}.
\]
AD_PROG = rosenbrock.cmp
AD_TOP = func
AD_IVARS = x
AD_DVARS = y
AD_PMAX = 2  # x has 2 elements
AD_OUTPUT_DIR = .

Figure 3.1. Example Script File (rosenbrock.adf)

The second form is used in defining list-valued options. Bindings may be provided as command line arguments and, additionally, as lines in a “script” file. Bindings specified as command line arguments to the preprocessor may contain whitespace, consisting of a sequence of spaces and tabs, if they are quoted.

A script file is a sequence of lines. Blank lines are ignored. Each nonblank line contains a binding having either of the two forms shown above. All characters on a line after the comment character ‘#’ are ignored. There is no formal requirement for the name of the script file, but our informal convention is to use the .adf extension. Bindings defined in script files may always use whitespace liberally.

All preprocessor options begin with an “AD_” prefix. Values of options are typically the names of files (AD_PROG), the name of a procedure in the program (AD_TOP), lists of names of variables in the program (AD_IVARS and AD_DVARS), integers (AD_PMAX), Boolean values (AD_DUMP_CALLGRAPH), and switches (AD_FLAVOR and AD_EXCEPTIONFLAVOR). For Boolean-valued options, FALSE, false and 0 are considered to be equivalent, as are TRUE, true and 1. Section 9 documents all of the ADIFOR Preprocessor options.

The ADIFOR Preprocessor processes bindings on its command line in the order that they are listed. As bindings are processed, new bindings always override values defined by a previous binding for the same option. The option AD_SCRIPT is used to specify the name of a script file. Whenever a binding for AD_SCRIPT is encountered, the file identified as the value of AD_SCRIPT is opened, and the bindings in the file processed in order.

Relative path names specified as command line arguments to the ADIFOR Preprocessor are taken as relative to the directory in which the preprocessor was executed. Relative path names specified in bindings specified in a script file are taken as relative to the directory containing the script file.

Now consider a sequence of examples using the script file rosenbrock.adf shown in Figure 3.1.

• Example 1

Adifor2.1 AD_PROG=rosenbrock.cmp AD_TOP=func \
    AD_DVARS=y AD_IVARS=x AD_PMAX=2 AD_OUTPUT_DIR=.

This command defines AD_PROG to be the filename “rosenbrock.cmp”, AD_TOP to be name of the procedure “func”, AD_IVARS to be the (single item) list “x”, AD_DVARS to be the (single item) list “y”, and AD_PMAX to be the integer value 2. ADIFOR will place derivative files in the current directory (which in UNIX is usually denoted by a dot).

• Example 2

Adifor2.1 AD_SCRIPT=rosenbrock.adf
This command defines exactly the same values for the same set of options.

- **Example 3**

```
Adifor2.1 AD_SCRIPT=rosenbrock.adf AD_PMAX=5
```

This command defines the exactly the same set of values for the same set of options, except for option `AD_PMAX` whose value is overridden with the integer value 5.

### 3.2 Compositions

Compositions list the names of all of the source files to be processed by the ADIFOR Preprocessor. A composition is a list of pathnames to source files with zero, one, or more pathnames per line. All characters on a line after the comment character ‘#' are ignored. Multiple pathnames on the same line are delimited by commas and whitespace, where whitespace is any sequence of spaces or tabs. Relative pathnames are taken to be relative to the directory containing the composition.

The name of the composition must end with a “.cmp” extension. The name of each source file must end with a “.f” suffix. Each source file listed in a composition may contain the source for one or more FORTRAN 77 routines.

A composition must be *top-complete* and *consistent*. To be top-complete, every routine that possibly by called as a result of invoking the top routine must be included in a source file listed in the composition. To be consistent, all procedure interfaces of routines in the listed source files must agree as to the number of arguments and the types of the arguments being passed. Many programs in use today have inconsistent interfaces. Fixing the inconsistencies may take significant effort, but is usually an enlightening process, resulting in a considerably more portable program.

In addition to being top-complete and consistent, your program must not be recursive. The ADIFOR Preprocessor will complain if it encounters a recursive program and will print out the names of each of the routines that are recursive. Recursion in FORTRAN 77 programs is usually, but not always, an indication of some underlying error.

When the ADIFOR Preprocessor generates derivative code for a file `somedir/foo.f`, it places the generated source code into a file `gfoo.f` in the subdirectory identified by the option `AD_OUTPUT_DIR` of the directory in which the preprocessor was executed. Therefore, no two pathnames listed in a composition may have the same basename, where the basename of `somedir/foo.f` is taken to be `foo.f`. The preprocessor will complain if multiple files in your program have the same basename.

### 3.3 Acceptable FORTRAN 77 Source Files

The ADIFOR Preprocessor recognizes standard FORTRAN 77 syntax extended with `DO-ENDDO`, `IMPLICIT NONE`, `DOUBLE COMPLEX`, and `INCLUDE`. Variable names need not be limited to six characters. If a program uses non-standard extensions, the preprocessor will probably not accept them. In particular, the preprocessor will not accept nonstandard intrinsic or type conversion functions, such as `arsin()`, `arcos()`, and `dfloat()`. These should be replaced with standard functions like `asin()`, `acos()`, and `dbles()`. In any case, for portability reasons, it is probably a good idea anyway to make sure that all code is standard-conforming. Also not accepted are system calls such as `etime()`. In most cases, such calls do not affect function evaluation and may be removed, commented out, or replaced with a syntactically correct but nonfunctional subroutine, prior to processing.

We strongly urge you to make sure that all of the files in your composition compile correctly and adhere to the FORTRAN 77 standard before submitting them to the ADIFOR Preprocessor for
processing. ADIFOR will complain about syntax errors, but its error messages are likely to be more cryptic. The preprocessor will also complain about problems in your source code that the typical FORTRAN 77 compiler will fail to identify, specifically, inconsistencies between callsites and the procedures they invoke, and inconsistencies between common block declarations across procedures.

For example, in the following program fragment an integer*4 array of length 3 is passed to a subroutine whose arguments were declared to be of type character*12.

```fortran
program main
  integer*4 x(3)
  ...
  call func(x)
  ...
end

subroutine func(c)
  character*12 c
  ...
end
```

The following program fragment declares common blocks to be of different length in different program units.

```fortran
program main
  call func1
  call func2
  ...
end

subroutine func1
  common /c10/ x(10)
  ...
end

subroutine func2
  common /c20/ x(20)
  ...
end
```

The FORTRAN 77 language definition requires that each common block, other than the blank common block //, must have the same size in each procedure in which it is declared. Another violation of the FORTRAN 77 standard in this program fragment is the fact that the common block is not declared in the main program from which both subroutines are called. While this is usually not an issue, because of the nature in which global variables are implemented, unexpected things could happen if a compiler exploited the liberty of the standard.
Chapter 4

A Tutorial Example

We demonstrate the use of ADIFOR 2.0 using the simple program shown in Figures 4.1 and 4.2. It shows a simple Newton iteration being used to minimize Rosenbrock’s function. The routines DLANGE and DGESV from the LAPACK package [1, 2] are used to compute the norm of $y$ and to solve the linear system $\frac{dy}{dx}s = -y$. Our goal will be to replace the subroutine $fprime$, which approximates $\frac{dy}{dx}$ by using central divided differences, with an ADIFOR-generated derivative code. This complete example is provided in $\$AD\_HOME/\texttt{examples/newton}$.

Rosenbrock’s function is used only for illustrative purposes. It is not indicative of the power of ADIFOR, which has processed programs up to 150,000 lines in length, albeit using more than 200 Mb of virtual memory in the process.

Step 1: Create a Composition File

Figure 4.3 presents composition $\texttt{rosenbrock.cmp}$ for the example, assuming that $\texttt{newton.func}$ and $\texttt{fprime}$ have been stored into the files $\texttt{newton.f}$, $\texttt{func.f}$, and $\texttt{fprime.f}$, and that code for $\texttt{dlange}$ and $\texttt{dgesv}$ and all of the routines that they invoke has been located.

Since $\texttt{func}$ does not invoke any other functions or subroutines, instead of tracking down all of the source code for $\texttt{dlange}$ and $\texttt{dgesv}$ and the routines they invoke, we are free to create a very short composition, $\texttt{rosenbrock-func-only.cmp}$ as shown in Figure 4.4, that contains only $\texttt{func.f}$.

Step 2: Create an ADIFOR Script File

To compute a Jacobian for the Newton example, you must provide ADIFOR with values for the following options:

$\texttt{AD\_PROG}$: The value of $\texttt{AD\_PROG}$ is the name of the “composition” to be processed. The name of the composition is communicated to the ADIFOR Preprocessor by specifying $\texttt{AD\_PROG=composition-name}$ on the command line.

In this example, $\texttt{AD\_PROG}$ will be set to $\texttt{rosenbrock.cmp}$.

$\texttt{AD\_TOP}$: The value of $\texttt{AD\_TOP}$ is the name of the procedure that contains the function to be differentiated. That procedure may invoke other procedures to an arbitrary nesting level. We refer to the procedure that is invoked to evaluate the function as the $\texttt{top-level\ routine}$ or $\texttt{TOP}$. The name of the procedure $\texttt{TOP}$ is communicated to the ADIFOR Preprocessor by using the command line option $\texttt{AD\_TOP=procedure-name}$. 

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PROGRAM NEWTON
DOUBLE PRECISION DUMMY,TOL, DLARGE
INTEGER INFO, N, IPIV(2)
DOUBLE PRECISION X(2),Y(2),YPRIME(2,2)
EXTERNAL DGESV, FPRIME, FUNC, DLARGE
TOL = 1.0E-12
WRITE (*,FMT=**) ’Input 2-element starting vector ’
READ (*,FMT=**) X(1),X(2)
CALL FUNC(X,Y)
10 IF (DLARGE(’1’,2,1,Y,2,DUMMY).LT.TOL) GO TO 20
   CALL FPRIME(X,Y,YPRIME)
   Y(1) = -Y(1)
   Y(2) = -Y(2)
   CALL DGESV(2,1,YPRIME,2,IPIV,Y,2,INFO)
   X(1) = X(1) + Y(1)
   X(2) = X(2) + Y(2)
   CALL FUNC(X,Y)
   WRITE (*,FMT=1000) ’Current Function Value:’,Y(1),Y(2)
   GO TO 10
20 CONTINUE
   WRITE (*,FMT=1000) ’Minimum is approximately:’,X(1),X(2)
1000 FORMAT (a,1x,2 (d15.8,2x))
END

Figure 4.1. A Simple Implementation of Newton’s Method

In Section 6 we will describe how to handle codes where the function to be differentiated does not conveniently correspond to a procedure invocation.

In this example, the function to be differentiated corresponds to the subroutine func, so we will set AD_TOP to be func.

AD_IVARS and AD_DVARS: The values of AD_IVARS and AD_DVARS are comma-separated lists of independent (input) and dependent (output) variables of TOP, respectively. AD_DVARS is a synonym for AD_DVARS. A variable may be designated as independent, dependent, or both (if it is overwitten during the execution of AD_TOP).

There is no way to nominate individual elements of a FORTRAN 77 array as being independent and dependent, although it is possible to specify at run time that only derivatives with respect to a particular set of elements should be computed (see Appendix A). Variables in the AD_IVARS and AD_DVARS lists must have type real, double precision, complex or double complex. The independent and dependent variables must be formal parameters of TOP or global variables declared within TOP. Again, in Section 6 we will describe how to handle codes in which the variables that logically correspond to the independent and dependent variables are neither formal parameters nor global variables in TOP.

In this example, in order to compute the derivatives of y with respect to x, we will set AD_DVARS to y and AD_IVARS to x.

AD_PMAX: The value of AD_PMAX is the upper bound on the number of independent variables for which derivatives can be computed simultaneously. It is necessary to specify this upper bound because FORTRAN 77 does not provide a standard mechanism for dynamic memory allocation. It is introduced as the first dimension of each of the gradient objects declared
SUBROUTINE FUNC(X,Y)
DOUBLE PRECISION X(2),Y(2)

Y(1) = 10.0 * (X(2)-X(1)*X(1))
Y(2) = 1.0 - X(1)
RETURN
END

SUBROUTINE FPRIME(X,Y,PRIME)
!
c approximates derivatives of Func by central differences.
c
C .. Array Arguments ..
DOUBLE PRECISION X(2),Y(2),DPRIPE(2,2)
C .. Local Scalars ..
DOUBLE PRECISION H
C .. Local Arrays ..
DOUBLE PRECISION XH(2),YM(2),YP(2)
C .. External Subroutines ..
EXTERNAL FUNC
C
IF (X(1).EQ.0.0) THEN
  H = 1.0e-7
ELSE
  H = X(1)*1.0e-7
END IF
XH(1) = X(1) - H
XH(2) = X(2)
CALL FUNC(XH,YM)
XH(1) = X(1) + H
XH(2) = X(2)
CALL FUNC(XH,YP)
YPRIPE(1,1) = (YP(1)-YM(1))/ (2.0*H)
YPRIPE(2,1) = (YP(2)-YM(2))/ (2.0*H)

IF (X(2).EQ.0.0) THEN
  H = 1.0e-7
ELSE
  H = X(2)*1.0e-7
END IF
XH(1) = X(1)
XH(2) = X(2) - H
CALL FUNC(XH,YM)
XH(1) = X(1)
XH(2) = X(2) + H
CALL FUNC(XH,YP)
YPRIPE(1,2) = (YP(1)-YM(1))/ (2.0*H)
YPRIPE(2,2) = (YP(2)-YM(2))/ (2.0*H)
RETURN
END

Figure 4.2. Rosenbrock’s Function and Divided-Difference Approximations of the Jacobian
newton.f
func.f
fprime.f

# LAPACK routines
dlange.f dgesv.f lsame.f dlssq.f
erbla.f dgetrf.f dgetsra.f ilaenv.f
dgetf2.f dlasp.f

# BLAS routines
dtrsm.f dgemm.f idamax.f dswap.f dscal.f dger.f

Figure 4.3. Composition for Newton’s Method Example (rosenbrock.cmp)

func.f

Figure 4.4. Composition for Newton’s Method Example (rosenbrock-func-only.cmp)

by the ADIFOR Preprocessor. The value of AD_PMAX is communicated by using the option
AD_PMAX=integer-value.

In the Newton example, we choose to set AD_PMAX to 2, since \( x \) is an array with 2 elements
and we would like to compute derivatives with respect to \( x(1) \) and \( x(2) \). In general, in the
invocation of the routines generated by the ADIFOR Preprocessor, we can use any value of
\( \text{g.p.} \) that is not larger than AD_PMAX. This issue is explained in more depth in Appendix A. We
also note that if subroutines using the same common blocks are processed separately with the
preprocessor, it is essential to use the same value of AD_PMAX in both cases, as otherwise the
gradient object common blocks are declared inconsistently.

AD_OUTPUT_DIR: The value of AD_OUTPUT_DIR specifies the name of the directory in which the ADIFOR
Preprocessor places the generated derivative code.

In the Newton example, we have chosen to set AD_OUTPUT_DIR to be “.” so that the generated
code will be placed back into the directory in which the ADIFOR Preprocessor is executed.

After determining the values for each of these options, create an ADIFOR script file containing
those values as shown in Figure 4.5.

AD_PROG = rosenbrock.cmp
AD_TOP = func
AD_IVARS = x
AD_DVARS = y
AD_PMAX = 2   # x has 2 elements
AD_OUTPUT_DIR = .

Figure 4.5. Script File for Newton’s Method Example (rosenbrock.adf)
subroutine g_func(g_p_, x, g_x, ldg_x, y, g_y, ldg_y)
double precision x(2), y(2)
C
integer g_pmax_
C
parameter (g_pmax_ = 2)
integer g_i_, g_p_, ldg_y, ldg_x
double precision d5_b, d2_b, g_y(ldg_y, 2), g_x(ldg_x, 2)
intrinsic dble
C
if (g_pmax_ .gt. g_p_) then
   print *, 'Parameter g_pmax_ is greater than g_p_'
   stop
endif
d2_b = dble(10.0)
d5_b = -d2_b * x(1) + (-d2_b) * x(1)
do g_i_ = 1, g_p_
g_y(g_i_, 1) = d5_b * g_x(g_i_, 1) + d2_b * g_x(g_i_, 2)
endo
y(1) = dble(10.0) * (x(2) - x(1) * x(1))
------
do g_i_ = 1, g_p_
g_y(g_i_, 2) = -g_x(g_i_, 1)
endo
y(2) = 1.0d0 - x(1)
------
return
end

Figure 4.6. The ADIFOR-generated Code for Subroutine func

Step 3: Invoke the ADIFOR Preprocessor

When executed with the command:

    Adifor2.1 AD_SCRIPT=rosenbrock.adf

the ADIFOR Preprocessor creates the subdirectory AD_cache, which contains internal information created by the preprocessor. Source files generated by the preprocessor are placed in the working directory. If AD_OUTPUT_DIR had been unspecified, then the default value of output_files would have caused the generated files to be placed into the subdirectory output_files. The preprocessor emits the augmented code for procedure func into the file g_func.f, whose source is shown in Figure 4.6. Note that usually an assignment statement in the original code has been replaced by a few assignment statements and a vector loop of length g_p_. When g_p_ is moderate, or the gradient objects always dense vectors, this is an efficient representation of this vector operation. The SparsLinC library (see Appendix C) provides an alternative approach for expressing this vector operation when the gradient objects are mostly sparse vectors.

Exactly the same processing process will be performed by executing the command:

    Adifor2.1 AD_PROG=rosenbrock.cmp AD_TOP=func \ 
    AD_DVARS=y AD_IVARS=x AD_PMAX=2 AD_OUTPUT_DIR=.

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but without the need to create `rosenbrock.adf`.

**Step 4: Incorporate ADIFOR-generated Subroutine**

Incorporating the ADIFOR-generated subroutine into a program to compute derivatives requires the following three steps:

1. **Allocate the gradient objects in the calling module.** The user should carefully check the ADIFOR-generated code to determine which variables in common blocks and which arguments to the top-level routine have been found to be active. For our small example, the declarations are

   ```plaintext
double precision g_x(PMAX,2), g_y(PMAX,2)
```

   where `PMAX` is an integer constant (FORTRAN 77 `PARAMETER`) whose value is greater than or equal to the value of `AD_PMAX`. In this case, we choose to set `PMAX` to 2.

2. **Initialize the seed matrix.** In order to compute the Jacobian of the function defined by `func`, the gradient object for the independent variable `x` should be initialized to a $2 \times 2$ identity matrix. This initialization amounts to saying that the derivative of each independent variable with respect to itself is 1.0.

3. **Call the ADIFOR-generated top-level subroutine.** The ADIFOR-generated subroutine computes both the function value and the value of the derivatives. So, in our example, we can replace the calls to `func` and `fprime` by a single call to `g_func`.

   In the call to the ADIFOR-generated top-level subroutine, the parameter `g_y` should be set equal to the length of the gradient objects, and all of the `1dg_` variables should be set equal to the leading dimension with which the corresponding gradient objects (`g_` variables) were actually declared. Thus, for our simple example, the call would look like

   ```plaintext
call g_func(2, x, g_x, PMAX, y, g_y, PMAX)
```

4. **Call the intrinsics error reporting routine.** `ehrpt` provides a summary report on FORTRAN 77 intrinsics that have been called at points where they are not differentiable. See appendix B for details.

For our example, the new driver is shown in Figure 4.7. As mentioned above, since ADIFOR-generated derivative code computes the transpose of the Jacobian, we must retranspose `g_y` before passing it to `dgesv`. Together with the subroutine `func` and the subroutine shown in Figure 4.6, the new program replaces the program shown in Figure 4.1.

**Step 5: Compile and Link**

After a suitable driver has been developed, the ADIFOR-generated code, the driver, and any other modules necessary to form a complete program should be compiled. Under UNIX, the necessary commands to compile and link an executable typically look like the following, where `f77` is the Fortran 77 compiler:

---

\(^1\)Some comments were removed to fit the program on one page.
PROGRAM ADNEWTON
C . Parameters .
INTEGER PMAX
PARAMETER (PMAX=2)
C . Local Scalars .
DOUBLE PRECISION DUMMY,TEMP,TOL
INTEGER INFO
C . Local Arrays .
DOUBLE PRECISION G_X(PMAX,2),G_Y(PMAX,2),X(2),Y(2)
INTEGER IPIV(2)
C . External Functions .
DOUBLE PRECISION DLANGE
EXTERNAL DLANGE
C .
TOL = 1.0E-12
WRITE (*,FMT=*) 'Input 2-element starting vector '
READ (*,FMT=*) X(1),X(2)
CALL FUNC(X,Y)
10 IF (DLANGE('1',2,1,Y,2,DUMMY).LT.TOL) GO TO 20
C compute function and Jacobian at current iterate
C
G_X(1,1) = 1.0
G_X(1,2) = 0.0
G_X(2,1) = 0.0
G_X(2,2) = 1.0
CALL G_FUNC(2,X,G_X,PMAX,Y,G_Y,PMAX)
C transpose g_y
C
TEMP = G_Y(2,1)
G_Y(2,1) = G_Y(1,2)
G_Y(1,2) = TEMP
C solve J * s = -f and update x = x + s
C
Y(1) = -Y(1)
Y(2) = -Y(2)
CALL DGESV(2,1,G_Y,PMAX,IPIV,Y,2,INFO)
X(1) = X(1) + Y(1)
X(2) = X(2) + Y(2)
C compute new function value
C
CALL FUNC(X,Y)
WRITE (*,FMT=1000) 'Current Function Value:',Y(1),Y(2)
GO TO 10
20 CONTINUE
WRITE (*,FMT=1000) 'Root is approximately:',X(1),X(2)
CALL EHRT
1000 FORMAT (a,1x,2 (d15.8,2x))
END

Figure 4.7. The Driver for the Newton Program Using ADIFOR-generated Code
f77 -c adnewton.f
f77 -c g_func.f
f77 -c dlan.ge.f
f77 -c dgesv.f
f77 -c ...
...
f77 -o adnewton adnewton.o g_func.o dlan.ge.o dgesv.o ...
  $AD_LIB/lib/ReqADIntrinsics-$AD_OS.o 
  $AD_LIB/lib/libADIntrinsics-$AD_OS.a

where the module ReqADIntrinsics-$AD_OS.o and archive libADIntrinsics-$AD_OS.a implement
the ADIFOR 2.0 exception handling packages. If the SparsLinC package is required, then it will be
necessary to link in the archive libSparsLinC-$AD_OS.a as well.

Under Windows 95/NT, the following commands should compile and link an executable, assuming that f132 is the Fortran 77 compiler:

f132 /c adnewton.f g_func.f 
  f132 /c dgemm.f dger.f dgesv.f dgetf2.f 
    dgetrf.f dgetrs.f dlan.ge.f dlassq.f 
    dlaswp.f dscal.f dsorm.f dtrsm.f 
    fprime.f xerbla.f func.f idamax.f 
    ilaenv.f lsame.f
  link *.obj %AD_LIB%\lib\ReqADIntrinsics.obj \ 
    %AD_LIB%\lib\ADIntrinsics.lib /out:adnewton.exe

where the module ReqADIntrinsics.obj and archive ADIntrinsics.lib implement the Windows 95/NT version of the exception handler package. If the SparsLinC package is required under
Windows 95/NT, then it will be necessary to link in the archive SparsLinC.lib.

See Appendix B for more information on the ADIntrinsics template expander and library. See
Section 8 if you encounter linking problems on a SPARC platform.
Chapter 5

Known Deficiencies

In this section we describe several deficiencies in ADIFOR 2.0’s support of full FORTRAN 77. In each case, it is relatively easy to “work around” each of these deficiencies. The ADIFOR Preprocessor flags each of these as being “not supported” any time that they are encountered.

5.1 Intrinsic s Passed as Procedure Parameters

The ADIFOR Preprocessor prohibits intrinsic s, such as DSIN and DCOS, from being passed as procedure parameters as shown in the standard-conforming FORTRAN 77 code:

```fortran
subroutine bad(x0, x1)
double precision x0, x1
external integrate
intrinsic dsin

call integrate(dsin,x0, x1)
end
```

This deficiency can easily be circumvented by introducing a wrapper function for each intrinsic, which is to be passed as a procedure parameter, and by then passing that wrapper routine as the procedure parameter instead of the intrinsic. For example, the following code performs the same computation as the code shown above by using a wrapper function MYDSIN for intrinsic DSIN:

```fortran
subroutine good(x0, x1)
double precision x0, x1
external integrate, mydsin

call integrate(mydsin, x0, x1)
end

function mydsin(x)
double precision x
intrinsic dsin
mydsin = dsin(x)
end
```
5.2 Intrinsics Overridden by External Functions

The ADIFOR Preprocessor prohibits external routines from overriding intrinsic functions as shown in the standard-conforming FORTRAN 77 code:

```
subroutine bad(x,y)
  external cos
  double precision x, y, cos
  c call user defined function with name "cos"
  y = cos(x0)
  end
  
  function cos(x)
  ...
  end
```

Again, this deficiency can easily be circumvented by renaming the external function so that it does not collide with the name of any intrinsic function, as follows:

```
subroutine good(x,y)
  external mycos
  double precision x, y, mycos
  y = mycos(x0)
  end

  function mycos(x)
  ...
  end
```

5.3 I/O Statements That Contain Function Invocations

ADIFOR Preprocessor prohibits I/O statements, i.e., READ, WRITE, and PRINT, from invoking functions and statement functions as shown in the standard-conforming FORTRAN 77 code:

```
subroutine bad(y)
  double precision y(10)
  integer f
  external f
  read (3, 50) x, y(f(x))
  50 format (...)
  end
```

Modifying code that invokes functions from within I/O statements is very easy, but may change the meaning of the I/O statements in ways that require other I/O statements in the program to be changed as well. For example, the function call in the READ statement above can be removed from an I/O statement by rewriting the code as follows:
subroutine okay(y)
double precision y(10)
integer f, i
external f
read (3, 50) x
i = f(x)
read (3, 51) y(i)
50 format (…)
51 format (…)
end

Notice, however, that in the original code, the two elements that are read come from the same input file record, while in the new code, the two elements come from different records.
Chapter 6

Advanced Topics

Normally, the ADIFOR Preprocessor assumes that independent variables are passed into the top-level routine \textbf{TOP}, and dependent variables are passed back out to the procedure that invoked \textbf{TOP}. Furthermore, it is assumed that the values of the independent variables will be assigned before \textbf{TOP} is invoked. “Passing” is either via procedure parameters or via global variables in common blocks. So, the normal ADIFOR 2.0 interface cannot compute derivatives of the following:

- variables that are declared and computed in the main program,
- variables that are declared locally in the top-level routine or variables declared in a routine transitively invoked by the top-level routine,
- variables that are assigned values during evaluation of \textbf{AD\_TOP} and then overwritten, and
- variables that are initialized by a \textbf{READ} statement.

This section describes some workarounds for these situations.

6.1 Computation Is Not Encapsulated in Procedure

Consider the following example:

```
program main
read(*,*) x(1)
t= result of some computation involving x(1)
read(*,*) x(2)
y= result of some computation involving x(1) and x(2)
end
```

To extract a procedure suitable for using ADIFOR 2.0 to generate code for \( \frac{\partial y}{\partial x(1)} \) and \( \frac{\partial y}{\partial x(2)} \), you should rearrange the computation so that both \( x(1) \) and \( x(2) \) are initialized first, then invoke a new procedure that computes \( y \) from \( x(1) \) and \( x(2) \) and then returns the value of \( y \) as follows:
**6.2 Variables Other Than Parameters and Globals in AD_TOP**

Consider the following program:

```fortran
program main
  call foo(x,y)
end

subroutine foo(x,y)
  a = x+1
  y = x*x
  b = x/2
end
```

If we want the derivative of \( y \) with respect to variable \( x \), the code is appropriate as is. But, if we want the derivatives of

- \( y \) with respect to variable \( a \),
- \( b \) with respect to variable \( x \), or
- \( b \) with respect to variable \( a \),

we run into a problem. Specifically, we cannot nominate a local variable of subroutine \texttt{foo} as dependent or independent, since it is not visible outside of \texttt{foo}. To avoid this problem, we make all “interesting” variables in subroutine \texttt{foo} visible through parameter passing or common blocks. For example, program \texttt{MAIN} could be rearranged to:

```fortran
program main
  call foo(x,y,a,b)
end

subroutine foo(x,y,a,b)
  a = x+1
  y = x*x
  b = x/2
end
```

or, alternatively,
program main
call foo(x,y)
end

subroutine foo(x,y)
common /globals/a,b
a = x+1
y = x*x
b = x/2
end

An alternative to this workaround is the buddy system discussed below.

6.3 Variables That Are Overwritten

Consider the following program:

program main
call foo(x,y)
end

subroutine foo(x,y)
10 y = x*x
20 y = y * x
end

Say we want to compute the derivatives with respect to \( x \) of variable \( y \) at both the statement with label 10 and the statement with label 20. Nominating variable \( y \) as the dependent variable, will generate code that computes only the derivative of \( y \) at the statement with label 20.

In order to avoid this problem, we can expand \( y \) into an array and modify the code to the code that follows:

program main
real y(2)
call foo(x,y)
end

subroutine foo(x,y)
real y(2)
10 y(1) = x * x
20 y(2) = y(1) * x
end

6.4 Variables Involved in I/O Statements

Sometimes the values of independent variables are read or computed within the active subtree (that is, within the subtree of procedures below the top-level subroutine). This procedure does not pose a problem, as long as the independent variables are parameters or global variables in \texttt{AD\_TOP}, and I/O functions are handled properly. Unfortunately, we cannot automate the proper handling of I/O
functions involving active variables because, in general, we have no way to trace the flow of data values that are read or written to files.

Without this information, we have no way of knowing whether the gradient object for a variable that is involved in a **READ** statement should be set to 0.0 or initialized by reading in derivative values from the file system. Similarly, we have no way of knowing whether we should write the values of the gradient objects for variables involved in a **WRITE** statement to the file system. Therefore, the ADIFOR Preprocessor currently just echoes I/O statements like **READ** and **WRITE** without introducing code to initialize or propagate the derivatives of variables involved in the I/O statement. Because of the problems that this approach may cause, the preprocessor generates a warning message whenever it processes a source file that contains an I/O statement involving an active variable. The warning message is printed out to **stderr** as the code is processed, and embedded as a comment just before the suspect I/O statement.

Fortunately, in most of the cases that we have encountered, it is possible to use a scheme based on “buddy variables” to modify the original function code in a manner that makes it possible for the ADIFOR Preprocessor to generate correct derivative code in the presence of I/O of active variables. This workaround was originally suggested by Andreas Griewank.

As an example, consider trying to process the following code to compute the derivative of **e** at the statement with label 20 with respect to **h** at the statement with label 10:

```
program main
  real lambda
  read *, lambda
  call foo(lambda)
end

subroutine foo(lambda)
  real lambda, e, h
  10  read *, h
      e = h * lambda
  20  write *, e
end
```

One approach to modifying this code would be to extract the **READ** statements in **foo** into **main**, and to convert variables **e** and **h** into parameters to **foo**. As an alternative, consider modifying the original code into the following code:
program main
real lambda, hbuddy, ebuddy
common /buddyvar/ hbuddy, ebuddy

read *, lambda
call foo(lambda)
end

subroutine foo(lambda)
real lambda, e, h, hbuddy, ebuddy
common /buddyvar/ hbuddy, ebuddy

h = 0
10 read *, h
   h = h + hbuddy
   e = h * lambda
   ebuddy = e
20 write *, e
end

and then nominating hbuddy as the independent variable, and ebuddy as the dependent variable. Initialization of hbuddy to 0.0 and g hbuddy to 1.0 in the derivative driver for g foo then results in g ebuddy being assigned the derivative of e with respect to h. Notice that nominating hbuddy and ebuddy as the independent and dependent variables forces variables h and e to be active. Since h is assigned the value 0.0 prior to the read statement, g h will be assigned the value 0.0. Therefore, since g hbuddy is initialized to 1.0, g h will be assigned the value 1.0 just after the READ, as required to compute the derivative of e with respect to h. Finally, the value of the computed derivative can be returned via the global variable g ebuddy.

The scheme that we just described has three key components. The first component forces variables in I/O statements that depend on the independent variables and that are used to compute dependent variables to be identified as active variables. The second component forces the derivatives of variables appearing in READ statements to be initialized properly. Finally, the third component makes it possible to retrieve the values of the derivatives for variables that appear in WRITE statements.
Chapter 7

Pitfalls of Differentiating FORTRAN 77

Some operations that are allowed in FORTRAN 77 do not have any (or, at least not the expected) mathematical meaning with respect to differentiation. Among these are:

- **Derivatives of integers and characters**

  The derivative of an integer or character is meaningless. As a consequence, if an integer is assigned a value from an active variable the integer variable does not become active. Thus, the gradient objects of any variables that depend on these integers may not have the expected values. The same holds true for characters.

- **Equivalencing of variables of different types**

  The process of equivalencing variables that have different types such as in the following code fragment

  ```fortran
  real r(10)
double precision d(5)
complex z(5)
equivalence(r,d)
equivalence(r,z)
  ```

  has no real mathematical meaning. Thus, if a program performs this operation, ADIFOR 2.0 will generate the corresponding *equivalences* for the gradient objects of the equivalenced variables, but they (and any gradient objects which depend on them) may have meaningless values. Note that this form of equivalencing is nonportable anyway, since its results depend heavily on the floating-point representation.

- **Introducing points of nondifferentiability**

  Sometimes, for the sake of improving efficiency, a program tests the value of a variable to see whether a function is being evaluated at a special point in space, and then computes the value of the function based on that knowledge. For example, the following piece of code computes $y = x^4$.
if ((x .eq. 0.0d0) .or. (x .eq. 1.0d0)) then
  y = x
else
  t = x*x
  y = t*t
endif

If automatic differentiation is used to compute \( \frac{dy}{dx} \), then the value of \( \frac{dy}{dx} \mid_{x=0} \) will be 1.0 (because the statement \( y = x \) implies that \( \frac{dy}{dx} = \frac{dx}{dx} = 1 \)) rather than the expected 0.0. Similarly, the value of \( \frac{dy}{dx} \mid_{x=1} \) will be 1.0 rather than 4.0. This “anomaly” stems from the fact that automatic differentiation differentiates the statements executed in the course of program execution. This issue, as well as other subtle pitfalls, is discussed in [16].
Chapter 8

Potential Problems

Users may encounter several problems while trying to process programs with ADIFOR 2.0. We provide a brief explanation of each and possible solutions.

- **ADIFOR 2.0 may complain about errors in the original FORTRAN 77 source code**
  As discussed in Section 3.3, ADIFOR 2.0 may report that errors are present in your FORTRAN 77 program that typical FORTRAN 77 compilers will not detect. Inconsistencies in subroutine interfaces and common blocks are the most frequently reported errors (see Section 3.3).

- **ADIFOR 2.0-generated code fails to link on a SPARC**
  Sun changed the interface to the internal I/O routines provided in libF77.a between versions SC1.0 and SC2.0 of the i77 compilation system. The default version of the ADIntrinsics library (suffix SunOS-4.x) that we provide has been compiled using version SC2.0. Unresolved references for entries beginning with three underscores, such as _do_1_in, _do_1_out, _e_rsle, _s_rsle, and _f_lushio, will be reported if you attempt to compile your source files with version SC1.0 and link against the SunOS-4.x libraries we provide. In this case, you should recompile the libraries (see section 2.2) and then link against them to build your executable.

- **ADIFOR 2.0 may generate subscripted variables with more than 7 dimensions**
  If the source code being differentiated contains active variables that are declared as arrays with 7 dimensions, then ADIFOR 2.0, when generating dense derivative code, will insert gradient objects with 8 dimensions. FORTRAN 77 limits the number of dimensions for arrays to 7. It is unlikely that you will run into this problem, but if you do, then check your compiler to see whether it has an option that will extend its limits.

- **ADIFOR 2.0 may generate variable names longer than 6 characters**
  ADIFOR 2.0 generates names for new variables that may be more than 6 characters long. FORTRAN 77 limits the number of characters in a name to 6, but all compilers we have worked with extend this limit. It is unlikely that you will run into this problem. If you do, then check your compiler to see whether it has an option that will extend its limits.

- **ADIFOR 2.0 generates DO-ENDDO loop statements instead of introducing a labeled CONTINUE statement to end each loop**
  The DO-ENDDO statement is not standard FORTRAN 77, but is accepted by all compilers that we have encountered.
• **Unneeded labels and continue statements appear in the ADIFOR-generated subroutines**

  In addition to creating new labels and continue statements, ADIFOR preserves those present in the original programs. There are two reasons for this functionality. The first reason is to ensure that any references to these labels (by a computed goto, for example) in the original program remain properly defined. Labels are also preserved to facilitate cross-referencing between the original and ADIFOR-generated code. If a certain algorithm is present near a particular label in the original program, it will be at the same location in the ADIFOR-generated code.

• **By default, ADIFOR 2.0 inserts variables whose names contain `.` characters**

  Some compilers may not permit `.` characters to appear in variable names. This problem can be avoided by setting the option **AD_SEP** to a character other than `.`.
Chapter 9

ADIFOR Preprocessor Options

This section provides short descriptions of each of the ADIFOR Preprocessor options. Default values for options are presented within square brackets. Options that can be defined with a list of values are identified with a “*” superscript.

9.1 Mandatory Options

- **AD_DVARS**
  List of names of the FORTRAN 77 variables that contain the dependent variables of the function to be differentiated. Synonym for AD_DVARS.

- **AD_IVARS**
  List of names of the FORTRAN 77 variables that contain the independent variables of the function to be differentiated.

- **AD_DVARS***
  AD_DVARS is a synonym for AD_DVARS. At least one of AD_DVARS and AD_DVARS must be defined.

- **AD_PMAX** (MANDATORY if AD_FLAVOR is dense)
  Maximum number of independent variables of the function to be differentiated. The value of this option is compiled into each of the dense derivative code files and is used as the first dimension of gradient objects for local and global variables.

- **AD_PROG**
  Name of composition file.

- **AD_TOP**
  Name of the top-level routine, the routine whose invocation is responsible for evaluating the function that is to be differentiated.

9.2 Other Options

- **AD_ACTIVATE_ALL [0]**
  If AD_ACTIVATE_ALL is true, then all floating point variables will be treated as being active.
• AD_ALL_SAVED [0]
  If your code assumes that all storage will be treated as static storage by your compiler, i.e., as
  if they had been listed in SAVE statements, then you must set AD_ALL_SAVED to true to generate
  correct derivative code. In this case, the ADIFOR Preprocessor will also treat all local and
global variables in your program as being static variables. Many FORTRAN 77 compilers treat
all local and global storage as being static, which means that variables always retain their value
between invocations of procedures. Use of this option will increase the time required for the
preprocessor to generate derivative code.

• AD_CACHE [AD_cache]
  Name of directory in which the ADIFOR Preprocessor stores information about your program
  as analysis is performed. Permits incremental reanalysis of your code after changes to the
  source code or changes in options.

• AD_CHECK_COMPOSITION [false]
  If set to true, the ADIFOR Preprocessor will check your program for syntax errors and
  inconsistent interfaces and then stop. Derivative code will not be generated.

• AD_DUMP_CALLGRAPH [false]
  If set to true, causes the ADIFOR Preprocessor to print out a callgraph for the program.

• AD_DUMP_INTERFACE [false]
  If set to true, then the ADIFOR Preprocessor will print out a description of each of the
  procedure interfaces in the program.

• AD_DUMP_INTERFACE2 [false]
  If set to true, then the ADIFOR Preprocessor will print out a description of each of the
  procedure interfaces in the program. The output format generated using AD_DUMP_INTERFACE2
  is somewhat different than that generated using AD_DUMP_INTERFACE.

• AD_EXCEPTION_FLAVOR [reportonce]
  May be set to terse, verbose, counting, performance, or reportonce to control level of
  exception handler error reporting. See Appendix B for more information.

• AD_EXCLUDE_PROCS []
  The ADIFOR Preprocessor ignores invocations of procedures listed in AD_EXCLUDE_PROCS, a
  comma-separated list of procedure names. Derivative code will not be generated for these
  procedures. Only use this option if the procedures you list are known not to impact the values
  of derivatives you want computed.

• AD_FLAVOR [dense]
  The ADIFOR Preprocessor generates dense derivative code (i.e., expressing gradient objects
  loops as normal FORTRAN 77 loops) if AD_FLAVOR is set to dense, and sparse derivative code
  (i.e., calls to the SparsLinC library) if it is set to sparse.

• AD_NAMESHIFT_CALLED_PROCS []
  The ADIFOR Preprocessor “shifts” the names of invoked procedures that appear in
  AD_NAMESHIFT_CALLED_PROCS, a comma-separated list of procedure names. The shifting oper-
  ation appends a suffix to the name of each listed procedure that encodes the type of each of
  its arguments.
- **AD_NAMESHIFT DEFINED_PROCS []**
  The ADIFOR Preprocessor “shifts” the names of defined procedures that appear in **AD_NAMESHIFT DEFINED_PROCS**, a comma-separated list of procedure names. The shifting operation appends a suffix to the name of each listed procedure that encodes the type of each of its arguments.

- **AD_NO_CLEANUP [false]**
  If **AD_NO_CLEANUP** is true then the ADIFOR Preprocessor will skip its “cleanup” phase. This is useful if you want to understand the hybrid mode of automatic differentiation, and code transformation, used by ADIFOR.

- **AD_NUM_RHS_VARS [5 if AD_FLAVOR is sparse, 500 if AD_FLAVOR is dense]**
  The ADIFOR Preprocessor transforms each assignment statement whose right-hand side expressions has more than **AD_NUM_RHS_VARS** into a sequence of simpler assignment statements.

- **AD_OUTPUT_DIR [output_files]**
  Directory into which the ADIFOR Preprocessor places the augmented source code files.

- **AD_PREFIX [g]**
  Character that serves as initial character of gradient object names and derivative computing procedure names. For example, by default, the gradient object for `foo` is `g_foo`.

- **AD_SCALAR_GRADIENTS [false]**
  If set to true and **AD_FLAVOR** is “dense”, then the ADIFOR Preprocessor will generate code that assumes that `g_pmax_` is 1. Executing this code provides an efficient means of generating `J*v`, where `J` is the Jacobian of the function being differentiated, and `v` is a vector.

- **AD_SCRIPT []**
  Name of file containing additional definitions of bindings.

- **AD_SEP [.]**
  Character that is used to separate components of generated variable names. If **AD_SEP** is changed to ‘$’, then the gradient object for `foo` will be named `g$foo`.

- **AD_SPARSLINCSUSE_64_PTR [false]**
  If **AD_FLAVOR** is `sparse`, then setting **AD_SPARSLINCSUSE_64_PTR** to `true` will cause the ADIFOR Preprocessor to declare derivative objects as INTEGER*8 values instead of INTEGER values. INTEGER*8 type variables should be able to contain all valid addresses on a 64-bit machine.

- **AD.Suppress_LDG [false]**
  If set to true and **AD_FLAVOR** is “dense”, then the ADIFOR Preprocessor will generate code that assumes that all gradient objects are allocated with first dimensions set to `g_pmax_`. Leading dimension arguments will not be passed as parameters throughout derivative code. Use of this option may allow the generated code to be vectorized efficiently.

- **AD.Suppress_NUM_COLS [false]**
  If set to true and **AD_FLAVOR** is “dense”, then the ADIFOR Preprocessor will generate code that assumes that `g_p_` is `g_pmax_`, and hence does not pass `g_p_` as a parameter throughout derivative code. Use of this option may allow the generated code to be vectorized efficiently.

- **AD_TEMPLATE_DIR []**
  Specifies an additional directory in which to search for ADIntrinsic template files. Only a single additional directory may be specified. See Appendix B for more information.
Appendix A

Seed Matrix Initialization

A.1 Introduction

This appendix focuses on the proper and efficient use of ADIFOR-generated codes through detailed examination of seed matrix initialization for the following cases:

- Dense Jacobian, one independent, one dependent variable
- Dense Jacobian, multiple independent, multiple dependent variables
- Sparse Jacobian, one independent, one dependent variable
- Sparse Jacobian, two independent variables, one dependent variable
- Partially separable functions

In most of these cases, a “variable” denotes an array; thus, we shall be dealing with vector-valued functions.

Note: The examples presented in Appendix A correspond to seed matrix initialization for the default or “nonsparse” flavor of ADIFOR 2.0 (see AD_FLAVOR in Chapter 9). The differences between the sparse and nonsparse ADIFOR 2.0-generated codes, which are discussed in Appendix C, impose differences in the mechanics of seed matrix initialization in each case (see Section C.4.4 for details). Nonetheless, the general seeding ideas presented here for the nonsparse case apply equally as well to the sparse case.

A.2 Case 1: Dense Jacobian, one independent, one dependent variable

Our first example is adapted from Problem C2 in the STDTST set of test problems for stiff ODE solvers [15] and was brought to our attention by George Corliss of Marquette University. The routine FCN2 computes the right-hand side of a system of ordinary differential equations \( \dot{y} = yp = f(x, y) \) by calling a subordinate routine FCN.

C File: FCN2.f

```fortran
SUBROUTINE FCN2(M,X,Y,YP)
INTEGER N
```
DOUBLE PRECISION X, Y(M), YP(M)
INTEGER ID, IWT
DOUBLE PRECISION W(20)
COMMON /STCOMS/W, IWT, N, ID

CALL FCN(X,Y,YP)
RETURN
END

C File: FCN.f

SUBROUTINE FCN(X,Y,YP)

C ROUTINE TO EVALUATE THE DERIVATIVE F(X,Y) CORRESPONDING TO THE
C DIFFERENTIAL EQUATION:
C DY/DX = F(X,Y).
C THE ROUTINE STORES THE VECTOR OF DERIVATIVES IN YP(*) . THE
C DIFFERENTIAL EQUATION IS SCALED BY THE WEIGHT VECTOR W(*)
C IF THIS OPTION HAS BEEN SELECTED (IF SO IT IS SIGNALLED
C BY THE FLAG IWT).

DOUBLE PRECISION X, Y(20), YP(20)
INTEGER ID, IWT, N
DOUBLE PRECISION W(20)
COMMON /STCOMS/W, IWT, N, ID
DOUBLE PRECISION SUM, CPARM(4), YTEMP(20)
INTEGER I, IID
DATA CPARM/1.D-1, 1.D0, 1.D1, 2.D1/

IF (IWT.LT.0) GO TO 40
DO 20 I = 1, N
  YTEMP(I) = Y(I)
  Y(I) = Y(I)*W(I)
20 CONTINUE
40 IID = MOD(ID,10)

C ADAPTED FROM PROBLEM C2
YP(I) = -Y(I) + 2.D0
SUM = Y(I)*Y(I)
DO 50 I = 2, N
  YP(I) = -10.0D0*I*Y(I) + CPARM(IID-1)*(2**I)*SUM
  SUM = SUM + Y(I)*Y(I)
50 CONTINUE

IF (IWT.LT.0) GO TO 680
DO 660 I = 1, N
  YP(I) = YP(I)/W(I)
  Y(I) = YTEMP(I)
660 CONTINUE
680 CONTINUE
RETURN
END

Most software for the numerical solution of stiff systems of ODEs requires the user to supply a
subroutine for the Jacobian of \( f \) with respect to \( y \). Such a subroutine can easily be generated by
ADIFOR. For the purposes of automatic differentiation, the vector \( Y \) is the independent variable, and the vector \( YP \) is the dependent variable. Then ADIFOR produces

```c
subroutine g_fcn2(g_p, m, x, y, g_y, ldg_y, yp, g_yp, ldg_yp)
C
C   ADIFOR: runtime gradient index
   integer g_p_
C   ADIFOR: translation time gradient index
   integer g_pmax_
   parameter (g_pmax_ = 20)
C   ADIFOR: gradient iteration index
   integer g_i_
C
C   integer ldg_y
   integer ldg_yp
   integer n
   double precision x, y(m), yp(m)
   integer id, iwt
   double precision w(20)
   common /stcom5/ w, iwt, n, id
C
C   ADIFOR: gradient declarations
   double precision g_y(ldg_y, m), g_yp(ldg_yp, m)
   if (g_p_.gt. g_pmax_) then
      print *, "Parameter g_p is greater than g_pmax."
      stop
   endif
   call g_fcn(g_p, x, y, g_y, ldg_y, yp, g_yp, ldg_yp)
   return

end
```

```c
subroutine g_fcn(g_p, x, y, g_y, ldg_y, yp, g_yp, ldg_yp)
C
C   ADIFOR: runtime gradient index
   integer g_p_
C   ADIFOR: translation time gradient index
   integer g_pmax_
   parameter (g_pmax_ = 20)
C   ADIFOR: gradient iteration index
   integer g_i_
C
C   integer ldg_y
   integer ldg_yp
C   ROUTINE TO EVALUATE THE DERIVATIVE \( F(X,Y) \) CORRESPONDING TO THE
C   DIFFERENTIAL EQUATION:
C   \( \frac{DY}{DX} = F(X,Y) \).
C   THE ROUTINE STORES THE VECTOR OF DERIVATIVES IN YP(*). THE
C   DIFFERENTIAL EQUATION IS SCALED BY THE WEIGHT VECTOR W(*)
C   IF THIS OPTION HAS BEEN SELECTED (IF SO IT IS SIGNALLED
C   BY THE FLAG IWT).
   double precision x, y(20), yp(20)
   integer id, iwt, n
   double precision w(20)
   common /stcom5/ w, iwt, n, id
   double precision sum, cparm(4), ytemp(20)
   integer i, iid
```
data cpam /1.d-1, 1.d0, 1.d1, 2.d1/
C
C //ADIFOR: gradient declarations
double precision g_ylgd_y, 20, g_yp1d_y, 20
double precision g_sum(g_pmax), g_yp(g_pmax, 20)
if (g_p_ .gt. g_pmax) then
  print *, "Parameter g_p is greater than g_pmax."
  stop
endif
if (iwt .lt. 0) then
  goto 40
endif
do 99999, i = 1, n
C
  ytemp(i) = y(i)
do g_i_ = 1, g_p_
    g_ytemp(g_i_, i) = g_y(g_i_, i)
  enddo
  ytemp(i) = y(i)
C
  y(i) = y(i) * w(i)
do g_i_ = 1, g_p_
    g_y(g_i_, i) = w(i) * g_y(g_i_, i)
  enddo
  y(i) = y(i) * w(i)
20 continue
99999 continue
40 iwt = mod(iwt, 10)
C
//ADAPTED FROM PROBLEM 2
C
yp1 = -y1 + 2.d0
do g_i_ = 1, g_p_
  g_yp(g_i_, 1) = -g_y(g_i_, 1)
  enddo
yp1 = -y1 + 2.d0
C
sum = y(i) * y(1)
do g_i_ = 1, g_p_
  g_sum(g_i_) = y(i) * g_y(g_i_, 1) + y(i) * g_y(g_i_, 1)
  enddo
sum = y(i) * y(1)
do 99998, i = 2, n
C
  yp1 = -10.0d0 * i * y(i) + cpam(iid - 1) * (2 ** i) * sum
  g_i_ = 1, g_p_
  g_yp(g_i_, 1) = cpam(iid - 1) * (2 ** i) * g_sum(g_i_) + -1
  *0.0d0 * i * g_y(g_i_, 1)
  enddo
  yp1 = -10.0d0 * i * y(i) + cpam(iid - 1) * (2 ** i) * sum
C
  sum = sum + y(i) * y(i)
do g_i_ = 1, g_p_
  g_sum(g_i_) = g_sum(g_i_) + y(i) * g_y(g_i_, i) + y(i) * g_y
  *(g_i_, i)
  enddo
  sum = sum + y(i) * y(i)
50 continue
99998 continue
if (iwt .lt. 0) then
  goto 680
endif
do 99997, i = 1, n
C
yp(i) = yp(i) / w(i)
do g_i = 1, g_p-
g_y(i, i) = (1 / w(i)) * g_y(g_i, i)
enddo
yp(i) = yp(i) / w(i)
C
y(i) = ytemp(i)
do g_i = 1, g_p-
g_y(i, i) = g_ytemp(g_i, i)
enddo
y(i) = ytemp(i)
660 continue
99997 continue
680 continue
return
end

The derivative objects \( g_y \) and \( g_{yp} \) are declared as matrices with 20 columns (since both \( y \) and \( yp \) were declared as vectors of length 20) and leading dimension 1dgy and 1dgyp respectively. The parameter \( g_p \) denotes the actual length of the gradient objects in a call to \( g_{fcn2} \). Since Fortran 77 does not allow dynamic memory allocation, derivative objects for local variables are statically allocated with leading dimension \( pmax \), whose value was selected by the user during the invocation of ADIFOR. A variable and its associated derivative object are treated in the same fashion; that is, if \( x \) is a function parameter, so is \( g_x \). Derivative objects corresponding to locally declared variables or variables in common blocks are declared locally or in common blocks as well.

Subroutine \( g_{fcn2} \) relates to the Jacobian

\[
J_{yp} = \begin{pmatrix}
\frac{\partial yp_1}{\partial y_1} & \cdots & \frac{\partial yp_1}{\partial y_m} \\
\vdots & \ddots & \vdots \\
\frac{\partial yp_m}{\partial y_1} & \cdots & \frac{\partial yp_m}{\partial y_m}
\end{pmatrix}
\]

as follows: Given input values for \( g_{p-}, m, x, y, g_y, 1dgy, \) and \( 1dgyp \), the routine \( g_{fcn2} \) computes both \( yp \) and \( g_{yp} \), where

\[
g_{yp}(1:g_{p-}1:m) = (J_{yp}(g_y(1:g_{p-}1:m))^T)^T.
\]

The superscript \( T \) denotes matrix transposition. The user must allocate \( g_{yp} \) and \( g_y \) with leading dimensions \( 1dgy \) and \( 1dgy \) that are at least \( g_{p-} \). While the implicit transposition may seem awkward at first, this is the only way to handle assumed-size arrays (like \( \text{real a(*)} \)) in subroutine calls.

Assume that \( m \) and \( g_{p} \) are 20 and that \( 1dgy \) and \( 1dgy \) are at least 20. Then we can compute the derivative matrix \( J_{yp} \) simply by initializing \( g_y \) to the identity:

**************
* Approach 1 *
**************

DO 10 I = 1, M
  DO 5 J = 1, M
  G_Y(I,J) = 0.0D
  5 CONTINUE
  G_Y(I,I) = 1.0D
10 CONTINUE
call g_fcn2(20, m, x, y, g_y, 1dgy, yp, g_yp, 1dgy)
On exit from $g.fcn2$, the variable $g\_yp$ contains the transpose of the Jacobian $J_{yp}$. Note that for this program to work, $g\_fn2$ must have been generated with AD\_PMAX at least 20.

Alternatively, we could have computed the Jacobian one column at a time:

```
***************
* Approach 2 *
***************
DO 10 I = 1, M
  * initialize first row of G_Y to i-th unit vector
  DO 5 J = 1, M
    G_Y(I,J) = 0.0D
  CONTINUE
  G_Y(I,I) = 1.0D0
  * call ADIFOR-generated derivative code
  call g\_fcn2(1, m, x, y, g\_y, ldg\_y, yp, g\_yp, ldg\_yp)
  * store ith column of the Jacobian in ith row of Jactrans array
  DO 15 J = 1, M
    JACTRANS(I,J) = G\_YP(I,J)
  CONTINUE
10 CONTINUE
```

Even though $g\_yp(i,j)$ as computed in Approach 1 equals $jactrans(i,j)$ computed in Approach 2, the second method is significantly less efficient. This inefficiency arises from the fact that the value of $yp$ itself is computed once in the first approach, but $m$ times in the second approach. Thus, it is usually best to compute as large a slice of the Jacobian as memory restrictions will allow. However, in this case, AD\_PMAX = 1 is sufficient, and, as a result, the memory requirements of the ADIFOR-generated code can be expected to be more modest, roughly 1/20th of the memory requirements of the previous code. In this fashion, the ADIFOR interface provides a mechanism for accommodating memory/runtime tradeoffs. An example of a parallel “derivative stripmining” technique based on this approach is presented in [9].

### A.3 Case 2: Dense Jacobian, multiple independent and multiple dependent variables

The second example involves a code that models adiabatic flow [25], a commonly used module in chemical engineering. This code models the separation of a pressurized mixture of hydrocarbons into liquid and vapor components in a distillation column, where pressure (and, as a result, temperature) decrease. This example was communicated to us by Larry Biegler of Carnegie-Mellon University.

In its original version, the top-level subroutine

```
subroutine aifl(kf)
 integer kf
```
has only one argument. All other information is passed in common blocks. For demonstration purposes, we changed the interface slightly to

```fortran
subroutine aifl(kf, feed, pressure, liquid, vapor)
    integer kf
    real feed(*), pressure(*), liquid(*), vapor(*)
```

copying the values passed in those arguments into the proper common blocks in `aifl`. As our first example, assume that we are interested in \( \frac{\partial \text{liquid}}{\partial \text{feed}} \) and \( \frac{\partial \text{vapor}}{\partial \text{feed}} \). In this case, ADIFOR generates

```fortran
subroutine g_aifl(g_p_, kf, feed, g_feed, ldg_feed, pressure,
    $    liquid, g_liquid, ldg_liquid,
    $    vapor, g_vapor, ldg_vapor)
    integer g_p_, kf, ldg_feed, ldg_liquid, ldg_vapor
    real feed(*), g_feed(ldg_feed,*), pressure(*),
    $    liquid(*), g_liquid(ldg_liquid,*),
    $    vapor(*), g_vapor(ldg_vapor,*)
```

In our example, the feed was a mixture of the hydrocarbons N-butane, N-pentane, 1-butene, cis-2-butene, trans-2-butene, and propylene, so the length of `feed`, `liquid`, and `vapor` was six, with `feed(1)` corresponding to the N-butane feed, and so on. If we set \( g_p = 6 \) and initialize `g_feed` to a \( 6 \times 6 \) identity matrix, then on exit `g_liquid(i,j)` contains

\[
\frac{\partial (\text{component } j \text{ in liquid})}{\partial (\text{component } i \text{ in feed})},
\]

which predicts by what amount the liquid portion of substance \( j \) will change if the feed of component \( i \) changes.

Suppose that we also wish to treat the pressure at the various inlets as being independent, and (because of the conservation law) decide not to declare "vapor" as being dependent, ADIFOR generates

```fortran
subroutine g_aifl(g_p_, kf, feed, g_feed, ldg_feed,
    $    pressure, g_pressure, ldg_pressure,
    $    liquid, g_liquid, ldg_liquid, vapor)
```

The initialization is a little more complicated this time. Assuming that we have 3 feeds (so `pressure` has three elements), the total number of independent variables is \( 6 + 3 = 9 \). `g_liquid` measures the sensitivity of the 6 substances with respect to changes in the 9 independent variables. Thus,

\[
J_{\text{liquid}} = \begin{pmatrix}
\frac{\partial \text{liquid}}{\partial \text{pressure}} & \frac{\partial \text{liquid}}{\partial \text{feed}}
\end{pmatrix}
\]

is a \( 6 \times 9 \) matrix. ADIFOR computes

\[
g_{\text{liquid}} = \left( J_{\text{liquid}} \begin{pmatrix}
g_{\text{feed}^T} \\
g_{\text{pressure}^T}
\end{pmatrix} \right)^T.
\]

If we wish to compute the whole Jacobian \( J \), then

\[
\begin{pmatrix}
g_{\text{feed}^T} \\
g_{\text{pressure}^T}
\end{pmatrix}
\]

\(^1\text{Actually, it is sufficient to compute one or the other, since, because of conservation laws, } \frac{\partial \text{liquid}}{\partial \text{feed}} + \frac{\partial \text{vapor}}{\partial \text{feed}} \text{ equals the identity matrix.}
must be initialized to a $9 \times 9$ identity matrix. Thus, $g_{\text{feed}}^T$ must contain the first six rows of a $9 \times 9$ identity matrix (since there are six variables in the feed), and $g_{\text{pressure}}^T$ must contain the last three rows of a $9 \times 9$ identity matrix. This configuration is achieved by initializing

$$g_{\text{feed}} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \text{ and } g_{\text{pressure}} = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 0 & 0
\end{pmatrix}.$$  

A.4 Case 3: Sparse Jacobian, one independent, one dependent variable

From the previous discussion, ADIFOR may seem to be well suited for computing dense Jacobian matrices, but rather expensive for sparse Jacobians. A primary reason is that the forward mode of automatic differentiation upon which ADIFOR is mainly based (see [7]) requires roughly $g_{\mathbb{P}}$ operations for every assignment statement in the original function. Thus, if we compute a Jacobian $J$ with $n$ columns by setting $g_{\mathbb{P}} = n$, its computation will require roughly $n$ times as many operations as the original function evaluation, independent of whether $J$ is dense or sparse. However, it is well known [13, 17] that the number of function evaluations that are required to compute an approximation to the Jacobian by finite differences can be much less than $n$ if $J$ is sparse. Fortunately, the same idea can be applied to greatly reduce the running time of ADIFOR-generated derivative code as well. This section suggests a technique for exploiting sparsity in derivative computations if the sparsity pattern is known a priori. Appendix C describes the the SparsLinC library, which, in conjunction with ADIFOR 2.0, allows exploitation of sparsity without a priori knowledge, and even computes the sparsity pattern of the Jacobian as a byproduct of the derivative computation.

The idea is best understood with an example. Assume that we have a function

$$F = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}: x \in \mathbb{R}^4 \mapsto y \in \mathbb{R}^5$$

whose Jacobian $J$ has the following structure (symbols denote nonzeros, and zeros are not shown):

$$J = \begin{pmatrix}
\circ & \circ & \circ \\
\circ & \circ & \circ \\
\bigtriangleup & \bigtriangleup & \bigcirc \\
\bigtriangleup & \bigtriangleup & \bigcirc \\
\bigtriangleup & \bigtriangleup & \bigcirc
\end{pmatrix}.$$

That is, the function $f_1$ depends only on $x_1$, $f_2$ depends only on $x_1$ and $x_4$, and so on. The key idea in sparse finite difference approximations is to identify structurally orthogonal columns $j_i$ of $J$—that is, columns whose inner product is zero, independent of the value of $x$. In our example, columns 1
and 2 are structurally orthogonal, and so are columns 3 and 4. This means that the set of functions that depend nontrivially on \( x_1 \), and the set of functions that depend nontrivially on \( x_2 \) are disjoint.

To exploit this structure, recall that ADIFOR (ignoring transposes) computes \( J \cdot S \), where \( S \) is a matrix with \( g_p \) columns. For our example, setting \( S = I_{4 \times 4} \) will give us \( J \) at roughly four times the cost of evaluating \( F \), but if we exploit the structural orthogonality and set

\[
S = \begin{pmatrix}
1 & 0 \\
1 & 0 \\
0 & 1 \\
0 & 1
\end{pmatrix},
\]

the running time for the ADIFOR code is roughly halved. Note that the ADIFOR-generated code remains unchanged.

As a more realistic example, we consider the swirling flow problem, part of the MINPACK-2 test problem collection [3], which was made available to us by Jorge Moré of Argonne National Laboratory. Here we solve a nonlinear system of equations \( F(x) = 0 \) for \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \). The swirling flow code has the form

```fortran
subroutine dswirl3(nxmax,x,fvec,fjac,ldfjac,job,eps,nint)
integer nxmax, ldfjac, job, nint
double precision x(*), fvec(*), fjac(ldfjac,*), eps
```

Like all codes in the MINPACK-2 test collection, it is set up to compute the function values (in \( fvec \)) and, if desired, the analytic first-order derivatives (in \( fjac \)) as well. The vectors \( x \) and \( fvec \) are of size \( nxmax = 14 \times nint \). For example, for \( nint = 4 \), the Jacobian of \( F \) is of size \( nxmax = 56 \) and has the structure shown in Figure A.1.

![Figure A.1. Structure of the swirling flow Jacobian, n = 56](image)

The derivative subroutine produced by ADIFOR is

```fortran
subroutine g_dswrl3 (g_p, nxmax, x, lg_x, ldg_x,
$                fvec, g_fvec, lg_x,
$                fjac, ldfjac, 1, eps, nint)
```

50
If we initialize \( g_\mathbf{x} \) to a \( 56 \times 56 \) identity matrix, and let \( \text{ldg}_\mathbf{x} = 56 \), and if \( \text{ldg}_\mathbf{x} \) is at least 56, then on exit from \( g_{\text{dswr13}} \), \( g_{\text{fvec}} \) will contain the transpose of \( \frac{\partial f}{\partial \mathbf{p}} \), stored as a dense matrix. As it turns out, less than 7% of the total operations performed with gradient objects in the ADIFOR code involve nonzeros. On the other hand, by using a graph-coloring algorithm designed to identify structurally orthogonal columns (we used the one described in [12]), we can determine that this Jacobian can be grouped into 14 sets of structurally orthogonal columns, independent of the size of the problem. In our example, columns 1, 16, 31, and 51 were in the first group; columns 2, 17, 37, and 43 were in the second group; and so on. We can take advantage of this fact by initializing the first column of \( g_\mathbf{x}^T \) such that it has 1.0 in rows 1, 16, 31, and 51; by initializing the second column of \( g_\mathbf{x}^T \) such that it has 1.0 in rows 2, 17, 37, and 43; and so on. The structure of \( g_\mathbf{x}^T \) thus initialized is shown in Figure A.2 together with the resulting compressed Jacobian \( g_{\text{fvec}}^T \). Note that instead of \( g_{\text{p}} = 56 \) we now can get by with \( g_{\text{p}} = 14 \), a sizable reduction in cost.

![Figure A.2. Left: Structure of \((g_\mathbf{x})^T\) Right: Structure of \((g_{\text{fvec}})^T\)](image)

Assuming that \texttt{color}(i)\) is the “color” of column \( i \) of the Jacobian and that \texttt{nocolors} is the number of colors (in our example we had 14 colors), the following code fragment properly initializes \( g_\mathbf{x} \) calls \( g_{\text{dswr13}} \) to compute the compressed Jacobian, and then extracts the Jacobian.

```c
n = 14*nint
do i = 1, n
   do j = 1, nocolors
      g_\mathbf{x}(j,i) = 0
   enddo
   g_\mathbf{x}(\text{color}(i),i) = 1
enddo

call g_{\text{dswr13}} (nocolors, nxmax, \mathbf{x}, g_\mathbf{x}, pmax, + fvec, g_{\text{fvec}}, pmax, + fjac, ldijac, \text{job}, eps, nint)
```

\( \text{job} = 1 \) indicates that only the function value is to be computed in \( \text{dswr13} \).
nonzero(j,i) is TRUE if the (j,i) entry in the Jacobian is nonzero, and FALSE otherwise.

do i = 1, n
  do j = 1, n
    if (nonzero(j,i)) then
      jac(j,i) = g_fvec(color(i),j)
    else
      jac(j,i) = 0.0
    endif
  endo
endo

Experimental results using this approach on a suite of problems from the MINPACK test set collection are presented in [4, 10].

A.5 Case 4: Sparse Jacobian, two independent variables, one dependent variable

The coating thickness problem, conveyed to us by Janet Rogers of the National Institute of Standards and Technology, presents many alternatives for using ADIFOR-generated subroutines. The code for this problem is (in abbreviated form) shown below:

```fortran
SUBROUTINE fun(n,m,np,nq,
+    beta,xplusd,ldxp,
+    f,ldf)

  c Subroutine Arguments
  c     => n    number of observations
  c     => m    number of columns in independent variable
  c     => np   number of parameters
  c     => nq   number of responses per observation
  c     => beta current values of parameters
  c     => xplusd current value of independent variable, i.e., x + delta
  c     => ldxp leading dimension of xplusd
  c     <= f    predicted function values
  c     => ldf leading dimension of f

  c Variable Declarations
  INTEGER      i,j,k,ldf,ldxp,m,n,np,nq,numpars
  INTEGER      ia,ib
  DOUBLE PRECISION beta(np),f(ldf,nq),xplusd(ldxp,m)

  double precision par(20),fn(2)

  do 10 k=1,np
    par(k) = beta(k)
  10 continue

  do 100 i=1,n
    do 20 j=1,m
      par(np+j) = xplusd(i,j)
  20 continue
```

52
c compute function values (fn) given parameters (par)
call fnc(par,fn)

\[ f(i,1) = fn(1) \]
\[ f(i,2) = fn(2) \]

100 continue
return
derend

subroutine fnc(x,fn)
integer m,np,nq
parameter (np=8,m=2,nq=2)
integer i
double precision x(np+m),fn(nq)
double precision beta(np),xplusd(m)
do 10 i=1,np
    beta(i) = x(i)
10 continue
do 20 i=1,m
    xplusd(i) = x(np+i)
20 continue

c compute first of multi-response observations

\[ fn(1) = beta(1) \]
\[ + \quad + beta(2)*xplusd(1) \]
\[ + \quad + beta(3)*xplusd(2) \]
\[ + \quad + beta(4)*xplusd(1)*xplusd(2) \]

c compute second of multi-response observations

\[ fn(2) = beta(5) \]
\[ + \quad + beta(6)*xplusd(1) \]
\[ + \quad + beta(7)*xplusd(2) \]
\[ + \quad + beta(8)*xplusd(1)*xplusd(2) \]

return
derend

The special format of this code is due to its embedding in the ODRPACK software for orthogonal distance regression. We are interested in the derivatives of \( f \) with respect to the variables \( \text{beta} \) and \( \text{xplusd} \). We shall explore various ways to do this in some detail.

**A.5.1 Approach 1 – Generate derivatives only for fnc**

The easiest approach is to generate the derivative code only for \( \text{fnc} \), since it is clear from the code that \( f(i,1:2) \) depends only on \( \text{beta}(1:np) \) and \( \text{xplusd}(i,1:m) \). ADIFOR then produces

```
subroutine g_fnc(g_p_, x, g_x, ldg_x, fn, g_fn, ldg_fn)
integer m, np, nq
parameter( np = 8, m = 2, nq = 2)
```
double precision $x(np+m)$, $fn(nq)$, $g_x(ldg_x,np+m)$, $g_{fn}(ldg_{fn},nq)$

If inside $fun$ we replace the call to $fnc$ with a call to $g_{fnc}$, always initializing $g_x$ to a $10 \times 10$ identity matrix before the call, then

$$g_{fn}(k,j) = \frac{\partial f(i,j)}{\partial beta(k)}, \quad k = 1, \ldots, 8, j = 1, 2.$$  

and

$$g_{fn}(k,j) = \frac{\partial f(i,j)}{\partial \text{plusd}(i,k-np)}, \quad k = 9, 10.$$  

Closer inspection reveals that the $10 \times 2$ array $g_{fn}$ always has the following structure (numbers are used to uniquely identify nonzero elements):

$$
\begin{pmatrix}
1 & 0 \\
2 & 0 \\
3 & 0 \\
4 & 0 \\
5 & 0 \\
6 & 0 \\
7 & 0 \\
8 & 0 \\
9 & 10 \\
11 & 12
\end{pmatrix}
$$

In other words, $fn(i,1)$ depends only on $beta(1:4)$, and $fn(i,2)$ depends only on $beta(5:8)$. Hence, we can compute a compressed version of $g_{fn}$ at reduced cost by merging rows 1 and 5, 2 and 6, 3 and 7, and 5 and 8 of $g_{fn}$. Keeping in mind that $g_{fn}$ is the transpose of the Jacobian, this is an especially simple case of the compression strategy outlined in the preceding section. This is achieved by initializing

$$g_x = 
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix},
$$

which results in

$$g_{fn} =
\begin{pmatrix}
1 & 5 \\
2 & 6 \\
3 & 7 \\
4 & 8 \\
9 & 10 \\
11 & 12
\end{pmatrix}.
$$

All the nonzero values of the Jacobian are now computed at roughly 60% of the cost of the previous approach.

On a SPARC-compatible Solbourne 5E/900 with a clock resolution of 0.01 seconds, executing $fun$ took 0.01 seconds, computing derivative values using $g_{fnc}$ without compression took 0.06 seconds, and exploiting the structure of $g_{fn}$ through the initialization of $g_x$ shown above reduced that time to 0.03 seconds.
A.5.2 Approach 2 – Generate derivatives for \texttt{fun}

An alternative method of applying ADIFOR is to process subroutine \texttt{fun}. ADIFOR detects the interprocedural data dependence between \texttt{fun} and \texttt{fnc} and therefore generates \texttt{g\_fun} as well as \texttt{g\_fnc}, with \texttt{g\_fnc} called properly within \texttt{g\_fun}. We obtain

```fortran
subroutine g\_fun(g\_p, n, m, np, nq, beta, g\_beta, ldg\_beta,
                $ xplusd, g\_xplusd, ldg\_xplusd, ldxdp, f, g\_f, ldg\_f, ldf)
integer g\_p, n, m, np, nq, ldg\_beta, ldg\_xplusd, ldxdp, ldg\_f, ldf
double precision beta(np), g\_beta(ldg\_beta, np),
                $ xplusd(ldxdp, m), g\_xplusd(ldg\_xplusd, ldxdp, m),
                $ f(ldf, nq), g\_f(ldg\_f, ldf, nq)
```

Now we have three-dimensional derivative objects, which somewhat complicates the initialization of \texttt{g\_xplusd} and the interpretation of the results in \texttt{g\_f}. However, this is not too difficult if we keep in mind that we wish to initialize

\[
\begin{pmatrix}
    \text{g\_beta}^T \\
    \text{g\_xplusd}^T
\end{pmatrix}
\]

to an identity matrix. The number of elements in \texttt{xplusd} is \(n \times m\), and the number of elements in \texttt{beta} is \(np\). For the coating thickness problem, \(n=63\), \(m=2\), and \(np=8\). Hence, the identity matrix should be \(134 \times 134\). This is also the value we shall use for \texttt{g\_p}. Initialization of \texttt{g\_beta} follows the scheme outlined in Section A.3; that is, the first 8 rows should be an \(8 \times 8\) identity matrix, and the remaining 126 rows should be initialized to zero. How to initialize \texttt{g\_xplusd} is less readily apparent, for it is not immediately obvious how to form a \(126 \times 126\) identity matrix from a three-dimensional structure. However, if one looks at the way Fortran stores two-dimensional structures in memory, a simple scheme for storing the Jacobian develops. In Fortran, element \((j, i)\) in an \(n \times m\) array is stored as if it were element \(n \times (i - 1) + j\) of a one-dimensional array. Thus, we can apply this technique to map the 126 columns of the Jacobian that should be initialized to the identity onto \texttt{g\_xplusd}. Specifically, element \((np + k, j, i)\) is initialized to 1 if and only if \(k = 63 \times (i - 1) + j\). The following code segment accomplishes this initialization.

```fortran
c n=63, m=2, np=8

\texttt{g\_p} = np + m*\texttt{n}
do 44 i = 1, np
  do 144 j = 1, \texttt{g\_p}
    g\_beta(j, i) = 0.0
  144 continue
  g\_beta(i, i) = 1.0
44 continue
do 45 i = 1, m
  do 145 j = 1, \texttt{n}
    do 245 k = 1, \texttt{g\_p}
      g\_xplusd(k, j, i) = 0.0
    245 continue
    g\_xplusd(np + (i-1)*\texttt{n} + j, j, i) = 1.0
145 continue
45 continue
```

When initialized in this manner, ADIFOR computes
\[
g_{f} = \left( J_f = \left( \frac{\partial f}{\partial \beta}, \frac{\partial f}{\partial x^{plusd}} \right) \right)^T.
\]

However, the performance of this approach is poor, since we totally ignore the sparsity structure of the Jacobian. As a result, the computation of \( J_f \) takes 0.77 seconds on a Solbourne 5E/900. A better way to find the Jacobian of \( f \) using \( g_{\text{fun}} \) is to take note of the structures used by \( \text{fun} \). From this, it becomes obvious that \( \frac{\partial f[j,k]}{\partial x^{plusd}[j]} \) is nonzero only when \( i = k \). As a consequence, we may change the

\[
g_{p} = np + m*n
\]

\[
g_{x^{plusd}}(np^+(i-1)*n)+j, j, i) = 1.0
\]

to the much simpler

\[
g_{p} = np + m
\]

\[
g_{x^{plusd}}(np^+i, j, i) = 1.0
\]

with the understanding that \( g_{f}(np^+i, j, k) \) \((i = 1...m)\) represents \( \frac{\partial f[j,k]}{\partial x^{plusd}[j]} \). This is equivalent to initializing

\[
g_{\beta} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad \text{and } g_{x^{plusd}}[n] = \begin{pmatrix}
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 0 \\
1 & 0 \\
0 & 1
\end{pmatrix}.
\]

This implementation is much more efficient than that described in the preceding paragraph and more closely mimics the behavior of the original subroutine \( \text{fun} \). As a consequence, the time required to execute \( g_{\text{fun}} \) using this initialization is 0.07 seconds.

As discussed in Section A.5.1, only half of the derivatives of \( f \) with respect to \( \beta \) are nonzero. Specifically, \( \frac{\partial f[j,k]}{\partial \beta(j)} \) is nonzero for \( j = 1.4 \) and zero for \( j = 5.8 \), while \( \frac{\partial f[j,k]}{\partial \beta(4)} \) is zero for \( j = 1.4 \) and nonzero for \( j = 5.8 \). This information can be used to further compress the Jacobian. The initialization

\[
g_{\beta} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad \text{and } g_{x^{plusd}}[n] = \begin{pmatrix}
0 & 0 \\
0 & 0 \\
0 & 0 \\
1 & 0 \\
0 & 1
\end{pmatrix}.
\]
compresses the Jacobian into only 6 columns. Columns 1 through 4 represent the nonzero derivatives of \( f \) with respect to \( \text{beta} \), while columns 5 and 6 correspond to the derivatives of \( f[i,j] \) with respect to \( \text{xp plusd}[i,1..2] \), as above. This initialization may be accomplished with the following code fragment.

```c
n=63, m=2, np=8
  halfnp = 4
  go 44 i = 1, halfnp
      go 144 j = 1, g_p-
          g_beta(j,i) = 0.0
          g_beta(j,i+halfnp) = 0.0
    144 continue
    g_beta(i,i) = 1.0
    g_beta(i,i+halfnp) = 1.0
44 continue
    go 45 i = 1, m
    go 145 j = 1, n
        go 245 k = 1, g_p-
            g_xplusd(k,j,i) = 0.0
      245 continue
    g_xplusd(halfnp+i,j,i) = 1.0
145 continue
45 continue
```

This approach is efficient, capable of computing all derivatives in 0.03 seconds. However, it has the disadvantage that the initialization routine might have to be changed if \textbf{fnc} or \textbf{np} is altered.

### A.6 Computing Gradients of Partially Separable Functions

A particular class of functions that arises often in optimization contexts is that of the so-called partially separable functions [14, 19, 20, 21, 22]. That is, we have a function \( f : \mathbb{R}^n \to \mathbb{R} \) that can be expressed as

\[
f(x) = \sum_{i=1}^{n_f} f_i(x).
\]

Usually each \( f_i \) depends on only a few (say, \( n_i \)) of the \( x \)'s, and one can take advantage of this fact in computing the (sparse) Hessian of \( f \).

As was pointed out to us by Andreas Griewank, now at the University of Dresden, this structure can be used advantageously in computing the (usually dense) gradient \( \nabla f \) of \( f \).

Assume that the code for computation of \( f \) looks as follows:

```fortran
subroutine f(n,x,fval)
  integer n
  real x(n), fval, temp

  fval = 0

  call f1(n,x,temp)
  fval = fval + temp
```
.....
call fnb(n,x,temp)
fval = fval + temp
return
end

If we submit $f$ to ADIFOR, it generates

$$
\text{subroutine g}_\text{fn} (g\_p\_, n, x, g\_x, \text{ldg\_x}, f\text{val}, g\_f\text{val}, \text{ldg\_fval}).
$$

To compute $\nabla f$, the first (and only) row of the Jacobian of $f$, we set $g\_p\_ = n$ and initialize $g\_x$ to a $n \times n$ identity matrix. Hence, the cost of computing $\nabla f$ is of the order of $n$ times the function evaluation.

As an alternative, we realize that with $f : \mathbb{R}^n \rightarrow \mathbb{R}^{nb}$ defined as

$$
g = \begin{pmatrix} f_1 \\ \vdots \\ f_{nb} \end{pmatrix},
$$

we have the identities

$$
f(x) = e^T g(x), \quad \text{and hence } \nabla f(x) = e^T J_g,
$$

where $e$ is the vector of all ones, and $J_g$ is the Jacobian of $g$. We can get the gradient of $f$ by computing $J_g$ and adding up its rows. The corresponding code fragment for computing $f$ is

```
subroutine f(n,x,fval)
integer n
real x(n)

integer nf, i
parameter (nf = <whatever>)
real gval(nf)

call g(n,x,gval)

fval = 0
do i = 1,nb
   fval = fval + gval(i)
endo

return
end
```

It may not appear that we have gained anything, since $J_g$ is $nf \times n$. If we initialize $g\_x$ in

$$
\text{subroutine g\_g (g\_p\_, n, x, g\_x, ldg\_x, gval, g\_g\text{val}, ldg\_g\text{val})}
$$
to an $n \times n$ identity matrix, then the computation of $J_g$ still takes about $n$ times as long as the computation of $g$ (or $f$).
The key observation is that the Jacobian $J_g$ is likely to be sparse, since

$$J_g = \begin{pmatrix}
(\nabla f_1)^T \\
\vdots \\
(\nabla f_n)^T
\end{pmatrix},$$

and each of the $f_i$'s depends only on $n_i$ of the $x$'s. By using the graph coloring techniques described in Section A.4, we can compute $J_g$ at a cost that is proportional to the number of columns in the compressed $J_g$, and then add up its (sparse) rows. As a result, we can compute $\nabla f$ at a cost that is potentially much less than $n$ times the evaluation of $f$. Alternatively, we can employ the SparseLinC library (see Appendix C), which will exploit sparsity even if the Jacobian contains a few dense rows (in this case, its chromatic number is $n$, and nothing has been gained). Experimental results with partially separable functions from the MINPACK test set collection are presented in [5].

Appendix B

ADIntrinsics 1.5: Exception Handling Support for ADIFOR 2.0

B.1 Introduction

In ADIFOR parlance, an “exception” is an event that occurs when an elementary function is evaluated at a point where the function result is defined, but the derivative is not. For instance, the square root of zero is zero, but the derivative of the square root function at zero is not defined. For most functions, there are several reasonable interpretations of what should be done when an exception occurs.

ADIFOR 2.0, by default, chooses the approach that was deemed appropriate for most cases, based on the arguments presented in [8, 23]. However, only a person familiar with the code can decide whether this choice is the correct one for a particular given instance. Hence, when an exception occurs, one should examine the derivative code generated by ADIFOR 2.0 to make sure that the default values had the desired effect. Section B.2 describes what every user should do to be aware of the occurrence of such exceptions. Section B.3 defines exceptional occurrences in ADIFOR 2.0 and the default action taken.

In dealing with FORTRAN 77 intrinsics, the ADIFOR 2.0 system relies on the ADIntrinsics system which has been developed mainly so that a user can easily customize the behavior of ADIFOR in the cases where the default option turns out to be inappropriate. It allows the user to specify alternative strategies through directives in the code to be differentiated and alternate template files, thereby documenting the changes and obviating the need to manually post-process the ADIFOR-generated code. The ADIntrinsics system also allows one to switch between different error reporting flavors. To achieve this flexibility, derivative code generation in ADIFOR 2.0 is split into two phases:

1. ADIFOR 2.0 generates code containing invocations of “templates” at call sites of FORTRAN 77 intrinsics. This code is contained in the files with the .A suffix in the AD_OUTPUT_DIR directory.

2. The purge postprocessor expands the templates into explicit Fortran code.

These two steps are usually transparent to users as these two components are invoked directly by the Adifor2.0 command. Section B.4 describes the different exception handler modes in details.

To link ADIntrinsics into your executable, you must add one of the following to your link line:

```
... $AD_LIB/lib/ReqADIntrinsics-$AD_OS.o \
   -L $AD_LIB -lADIntrinsics-$AD_OS # in UNIX
```
or

```bash
... $AD_LIB/lib/ReqADIntrinsics-$AD_OS.o \\
$AD_LIB/lib/libADIntrinsics-$AD_OS.a # in UNIX
```
or

```bash
... %AD_LIB%/\lib\ReqADIntrinsics-%AD_OS%.obj \\
%AD_LIB%/\lib\libADIntrinsics-%AD_OS%.lib # in Windows^95/NT
```

The reason for not combining the two files in one archive is that the .o file contains some block data initializations which may not get linked into your executable if they are contained in the archive.

In section B.5, we describe how to change the exception reporting options, such as, for example,

1. changing the exception handler output unit,
2. resetting the exception handler counts,
3. dynamically changing between different levels of exception reporting, or
4. ignoring exceptions in particular regions of code.

5. Section B.6 describes how to redefine the exceptional values returned at points of nondifferentiability, either by changing globally the definitions of default values for certain exception classes, or by changing the behavior associated with a particular intrinsic.

Lastly, in Section B.7, we present an example of employing some of these features. We also mention that the user can go beyond what is described here in redefining the behavior of the exception handler by redefining the templates governing the parse translation. These issues will be described in a forthcoming edition of this user guide.

### B.2 What Every User Should Do

To obtain a summary report on intrinsic exceptions, one should *always* call the routine `ehrpt` (for exception handler report) after the call to the ADIFOR-generated procedure derived from the top-level subroutine.

```plaintext
program main
    [...] call ADIFOR_GENERATED_CODE () [...] call EHRPT return end
```

### B.3 Definition of Intrinsic Exceptions and Default Behavior

Some of the FORTRAN 77 intrinsics are not globally differentiable at all points of their domain, such as, for example, \( \frac{d}{dx}\cot x \big|_{x=0} \). However, the propagation mechanism employed in automatic differentiation requires that *some value* be returned for that derivative. Table B.1 lists the five types of exceptional values employed, their default value (in brackets), and their interpretation.
<table>
<thead>
<tr>
<th>Exceptional Value [Default]</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>JumpVal[0]</td>
<td>The function is discontinuous at this point.</td>
</tr>
<tr>
<td>NoLimit[0]</td>
<td>The directional derivatives do not agree.</td>
</tr>
<tr>
<td>TieVal[0.5]</td>
<td>The case $x = y$ for $\min$ and $\max$.</td>
</tr>
<tr>
<td>InfVal[0]</td>
<td>The derivative approaches infinity.</td>
</tr>
<tr>
<td>NaNVal[0]</td>
<td>Not even a generalized interpretation makes sense.</td>
</tr>
</tbody>
</table>

Table B.1. Exceptional Derivative Values

<table>
<thead>
<tr>
<th>Intrinsic</th>
<th>$f_x$ undefined</th>
<th>Default Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>AINT(x)</td>
<td>$x = \pm 1, \pm 2, \ldots$</td>
<td>JumpVal</td>
</tr>
<tr>
<td>ANINT(x) and DNINT</td>
<td>$x =$ odd multiples of 1/2</td>
<td>JumpVal</td>
</tr>
<tr>
<td>ABS(x)</td>
<td>$x = 0$</td>
<td>NoLimit</td>
</tr>
<tr>
<td>MOD(x,y)</td>
<td>$x = n \times y$ for an integer $n$</td>
<td>JumpVal</td>
</tr>
<tr>
<td>SIGN(x,y)</td>
<td>$x = 0$ or $y = 0$</td>
<td>JumpVal</td>
</tr>
<tr>
<td>DIM(x,y)</td>
<td>$x = y$</td>
<td>NoLimit</td>
</tr>
<tr>
<td>MAX(x,y)</td>
<td>$x = y$</td>
<td>TieVal</td>
</tr>
<tr>
<td>MIN(x,y)</td>
<td>$x = y$</td>
<td>TieVal</td>
</tr>
<tr>
<td>SQRT(x) real-valued x</td>
<td>$x = 0$</td>
<td>InfVal</td>
</tr>
<tr>
<td>SQRT(x) complex-valued x</td>
<td>$x = 0$</td>
<td>NaNVal</td>
</tr>
<tr>
<td>ASIN</td>
<td>$</td>
<td>x</td>
</tr>
<tr>
<td>ACOS</td>
<td>$</td>
<td>x</td>
</tr>
</tbody>
</table>

Table B.2. Points of Nondifferentiability and Default Values of Partial for unary FORTRAN 77 Intrinsics

These default exceptional values are employed as shown in Tables B.2 and B.3. We employ the shorthand $f_x$ and $f_y$ to denote the partial derivative with respect to the first and second argument, respectively.

In case of a complex-valued argument, $\text{abs}(x)$ is treated like $\text{sqrt}(\text{re}(x)^2 + \text{im}(x)^2)$, and hence has the same exceptional behavior like the real-valued square root.

The following principles were considered in designing the ADIFOR exception-handling mechanism (see [8, 23] for more background information):

**Generalized Gradient:** Many algorithms for optimizing nonsmooth functions use generalized gradient values. A generalized gradient is any value in the convex hull of derivative values in the neighborhood of the point of nondifferentiability. For univariate functions, one may obtain any value in the interval $[\lim \inf f', \lim \sup f']$. For example, a generalized gradient for $|x|$ at 0 is any number in $[-1, 1]$. The values we choose to return as “derivative” values at points of nondifferentiability are generalized gradient values, provided that the chain rule for generalized gradients holds as a set inequality, rather than an inclusion [11].

**Continuity of Catastrophe:** The value at the point of nondifferentiability should in some sense be the limit of what happens in a neighborhood. For example, the derivative of $\text{asin} (x)$ at 1 should be $\text{INFINITY}$. For some functions, the mathematical limit may be different from the computational limit, as a result of finite precision or denormalized numbers.

**Extreme Point:** A necessary condition for the existence of an extreme point is $f' = 0$. A point of
nondifferentiability is usually at least a local extreme point, so returning a value of 0 as the
derivative may signal an optimization algorithm that an extreme point has been found.

**Evaluation of Undefined Functions:** In some computing environments, execution may continue
after an attempt to evaluate a function at a point outside its domain (perhaps with a value
of NaN). If the program has not crashed while evaluating $\sqrt{-2.0}$ (in real arithmetic), then our
derivative evaluation should not crash, either.

**Scaling:** It is critical to scale many applications appropriately before applying an optimization or
ODE-solving algorithm. In many calculations, variable vectors are scaled by their $L_2$ norm
or $L_\infty$ norm (i.e., the sum or maximum of the component moduli). Later on, this scaling
is undone so that the overall calculation is mathematically smooth, even when some of the
components are zero or their absolute values are tied at the maximum. The derivative is locally
not defined, but the entire computation is globally differentiable. We have attempted to return
derivative values that make sense in connection with commonly used scaling techniques.

These principles often conflict with one another and have different implications regarding the
values that should be returned at points of nondifferentiability. We made trade-off choices that we
think can be justified.

For `sqrt`, at the point of nondifferentiability $x = 0$, the default for `InfVal = 0` is a generalized
gradient value if we assume that `sqrt(x) := sqrt(abs(x))`. Further, it makes expressions like
`sqrt(X*X*Y + Y*Y*Y)` have the correct derivative. However, it violates the principle of
continuity of catastrophe. Alternatively, the value of `InfVal = INFINITY` makes the one-sided limit
correct. For `asin` and `acos`, at the points of nondifferentiability $x = \pm 1$, the default for `InfVal
= 0` indicates an extreme point. However, it violates the principle of continuity of catastrophe.
Alternatively, the value of `InfVal = INFINITY` makes the one-sided limit correct. If $|x| > 1$, usually
the user’s original code will have already crashed while evaluating `asin(x)`. If it has continued
execution (perhaps with value NaN), we should continue execution also. No value is reasonable since
the function is not defined, so we choose to return the same value as at $x = \pm 1$. Alternatively, we
could return whatever was assigned to the value of `asin(x)`.

For the `sign` function, at the point of nondifferentiability $x = 0$, the default value of 0 for
`NoLimit` is a generalized gradient value equal to the average of the two limits from each side. Using
`NoLimit = 0` also provides a generalized gradient for `abs` at the point of nondifferentiability $x = 0$
and indicates an extreme point. This choice also satisfies the generalized gradient requirement for
dim at the points of discontinuity, $x = y$.

The derivatives of `aint` and `anint` are set to `JumpVal` at the points of nondifferentiability, and
0 elsewhere. The default value for `JumpVal` is 0, the limit from each side. The derivative of `mod`
is also set equal to `JumpVal` at points of discontinuity. Although the default value of 0 is not equal to

<table>
<thead>
<tr>
<th>Intrinsic</th>
<th>$f_x$ undefined</th>
<th>Default for $f_x$</th>
<th>$f_y$ undefined</th>
<th>Default for $f_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOD(x,y)</td>
<td>$x = n \times y$ for an integer $n$</td>
<td>JumpVal</td>
<td>never</td>
<td>N/A</td>
</tr>
<tr>
<td>SIGN(x,y)</td>
<td>$x = 0$ or $y = 0$</td>
<td>JumpVal</td>
<td>never</td>
<td>N/A</td>
</tr>
<tr>
<td>DIM(x,y)</td>
<td>$x = y$</td>
<td>NoLimit</td>
<td>$x = y$</td>
<td>same as for $f_x$</td>
</tr>
<tr>
<td>MAX(x,y)</td>
<td>$x = y$</td>
<td>TieVal</td>
<td>$x = y$</td>
<td>$f_y = 1 - f_x$</td>
</tr>
<tr>
<td>MIN(x,y)</td>
<td>$x = y$</td>
<td>TieVal</td>
<td>$x = y$</td>
<td>$f_y = 1 - f_x$</td>
</tr>
<tr>
<td>$x^y$</td>
<td>$x = 0$ and $0 &lt; y &lt; 1$</td>
<td>InfVal</td>
<td>$x &lt; 0$ or ($x = 0$ and $y = 0$)</td>
<td>NoLimit</td>
</tr>
</tbody>
</table>
the limit from both sides, which is 1, it does signal an extreme value, important for optimization.

The default value for TieVal is 1/2. This value has the benefit that it is a generalized gradient and implies that if \( x = y \) then \( f_x = f_y \). However, Fortran’s \texttt{max} and \texttt{min} functions accept more than two arguments. Consequently, the current implementation of ADIFOR breaks all calls to \texttt{min} and \texttt{max} into a series of binary calls. Thus, if many arguments are equal, their slopes are weighted \( 1/2, 1/4, 1/8, \ldots \).

### B.4 Exception Handler Modes

The exception handler operates in five modes: verbose, report-once, counting, terse, and performance. The default mode is \texttt{reportonce}. Note, however, since \texttt{reportonce} requires the compilation of some C libraries, if your system does not support a C compiler, you will need to override this default by setting \texttt{AD\_EXCEPTION\_FLAVOR} to one of \texttt{performance}, \texttt{terse}, \texttt{counting}, or \texttt{verbose}.

In verbose mode, \textit{every time} an exceptional condition occurs, a message is written to the program’s error unit (by default unit number zero, which usually outputs to the screen) indicating the function, the arguments to the function, and the file name and line number containing this function evaluation. A sample output line is shown in Figure B.1. This information allows one to track down exactly where the exception is occurring and decide whether it is generating appropriate results. However, this option may generate a significant amount of output.

Report-once mode combines all of the exception reports for a source line into a single report, as shown in Figure B.2.

In addition, counting, terse, and performance modes provide a decreasing amount of information about exceptions that occur.

\textit{Note: Unless you invoke the exception handler reporting routine \texttt{ehrp}t after the execution of the ADIFOR-generated code, you will not see any of the reports generated by the report-once, counting, and terse modes.}

Counting mode maintains a running total of each \textit{type} of exception that occurs, as shown in Figure B.3. It avoids the work associated with tabulating exceptions in report-once mode, and hence should execute faster.

Terse mode indicates whether any exceptions of a given type occurred. This mode may be useful for vectorizing compilers, where the recurrence required for counting may inhibit vectorization. A sample terse mode output is given in Figure B.4.

Performance mode contains only a minimal amount of exception-checking code. It makes no subroutine calls and always assigns the default value when an exception occurs. We suggest that one should only use performance mode after running the code with report-once or verbose mode and convincing oneself that either no exceptions occur or the default exception handling is appropriate. The following sections describe how to change the default handling in case it is not. No report is made, since no exceptions are tracked.
At line 100 in file "g_func.f", while executing routine "foo", an exception occurred evaluating ABS : 50 times.

At line 3 in file "g_misc.f", while executing routine "bar", an exception occurred evaluating ABS : 1 time.

At line 7 in file "g_misc.f", while executing routine "bar", an exception occurred evaluating POWER: df/dx : 5 times.

At line 17 in file "g_misc.f", while executing routine "bar", an exception occurred evaluating ACOS first deriv : 17 times.

At line 920 in file "g_misc.f", while executing routine "bar", an exception occurred evaluating ABS : 49 times.

Figure B.2. Report-once Mode Error Report

Double precision exception(s) occurred evaluating:
ABS : 100 times.
POWER: df/dx : 5 times.
ACOS first deriv : 17 times.

Figure B.3. Counting Mode Error Report

Double precision exception(s) occurred evaluating:
ABS
POWER
ACOS first deriv

Figure B.4. Terse Mode Error Report
The exception handling mode may be chosen at the time ADIFOR 2.0 is executed by setting the AD_EXCEPTION_FLAVOR variable to one of: performance, terse, counting, reportonce, or verbose.

B.5 Changing Exception Reporting Options

B.5.1 Redirecting Exception Handler Output

Two different routines are provided for report-once mode and the remaining exception handling modes. Two different routines are necessary as report-once mode is generated by a C subroutine, whereas all other output modes are generated by Fortran code.

**Report-once Mode — ehofil:** To direct the output of report-once mode to a file, call ehofil with the name of the output file, e.g.,

```fortran
call ehofil ('reportonce.out')
```

**All Modes but report-once — ehsup:** To direct the exception handler output for all modes but report-once to a different unit, open the unit in your driver program, and then call ehsup with two parameters: -1, and then the unit number. The driver is also responsible for closing this unit before the program terminates. Failure to do so may result in a loss of output that has been buffered but not written to the file.

```fortran
call ehsup (-1, UNIT-NUMBER)
```

A segment of the user code might resemble this fragment.

```fortran
open (UNIT=13, FILE='adifor-errors.out')
call ehsup (-1, 13)
[... Useful Work ...]
close(13)
```

B.5.2 Resetting Exception Counts

The routine ehrst causes all counts of exceptions to be reset to zero. An example of use is

```fortran
call ehrst()
```

B.5.3 Fine-Grained Control of Exception Handler Modes

Fine-grained control over exception handler modes is achieved by embedding directives in the user’s code.

**Change of Verbosity Level:** The verbosity level can be dynamically set with the AD_EXCEPTION_LEVEL() directive. Valid levels are verbose, counting, terse, reportonce, performance, and default, which restores the exception level to the one with which ADIFOR 2.0 was run. For example, to guarantee verbose exception reporting around a certain region, the user might use the following code:
C    AD_EXCEPTION_LEVEL(VERBOSE)
     [... Interesting Code Here ...]
C    AD_EXCEPTION_LEVEL(DEFAULT)

Warning:
Terse mode is incompatible with both counting mode and verbose mode in the sense that
switching from verbose or counting mode to terse mode anywhere in your program leads
to incorrect summary information being reported by ehrpt.

If you intend to use the report-once mode anywhere in your program, you must run
ADIFOR 2.0 with the AD_EXCEPTION_FLAVOR=reportonce binding. Otherwise, report-
one mode will not function properly.

Ignoring Exceptions in a Region: To ignore exceptions in a region, bracket the region with
the directives AD_EXCEPTION_BEGIN_IGNORE and AD_EXCEPTION_END_IGNORE. “Ignoring” exceptions
simply means that no exceptional information is printed out; it does not mean that the exception
handler is disabled.¹ Truly disabling the exception handler (that is, using performance mode)
should be done with caution, because at exceptional points the performance mode may return a
value different than that returned by the exception handler for a user-configured value.

C    AD_EXCEPTION_BEGIN_IGNORE()
     [... Exceptions to be Ignored Here ...]
C    AD_EXCEPTION_END_IGNORE()

Warning: These directives do not nest. This means that any AD_EXCEPTION_END_IGNORE
cancels all previous AD_EXCEPTION_BEGIN_IGNORE commands, regardless of how many
preceded the end ignore.

Here is an example showing how the ignore directives do not nest.

C    AD_EXCEPTION_BEGIN_IGNORE()
     [... Exceptions are Ignored Here ...]
C    AD_EXCEPTION_BEGIN_IGNORE()
     [... Exceptions are Ignored Here ...]
C    AD_EXCEPTION_END_IGNORE()
     [... Exceptions are REPORTED Here ...]
C    AD_EXCEPTION_END_IGNORE()
     [... Exceptions Continue to be Reported Here ...]

Syntax of Directives: The syntax of the directives is intended to be reasonably intuitive:

- any comment character (C, c, or *) may be used to begin the comment line;
- spaces cannot appear in the middle of a keyword, but may appear around parentheses and
  commas;
- the directives can appear in upper or lower case, as can the keywords (arguments) given; and

¹Currently, the “ignore” mode is implemented by placing the exception handler in counting mode for the given
region.
• zero or more whitespace characters may appear between the comment character and the beginning of the directive, but no other spurious characters should appear in the line, even after column 72.

Warning: Directives affect only the parts of the program that are literally after them. In particular, a directive cannot change the mode in which an invoked procedure runs. The example below shows incorrect usage of the AD_EXCEPTION_LEVEL directive.

C This is an incorrect use of the AD_EXCEPTION_LEVEL directive.
C it has no effect on the subroutine "slow_func".
C
C AD_EXCEPTION_LEVEL(PERFORMANCE)
call slow_func
C AD_EXCEPTION_LEVEL(DEFAULT)

B.6 Modifying Exceptional Behavior

For each of the FORTRAN 77 intrinsics that are not globally differentiable, 

purse requires a default value to be inserted for the first (and sometimes also second) partial derivatives at the point of nondifferentiability.

It is possible to override the default behavior for the exceptions. This overriding is precision-specific, and is done through the routines ehsev* and ehsup*, where * is one of s, d, c, or z, for single, double precision, complex, or double complex, respectively. The first one changes the values associated with the symbolic exception values InfVal, etc. (see section B.3), the second changes the exceptional behavior associated with a particular intrinsic function.

B.6.1 Changing Exception Class Default Values

The routines ehsev*, where * is one of s, d, c, or z, for single, double precision, complex, or double complex, respectively, allow the user to set the symbolic exceptional values “InfVal”, “NaNval”, “NoLimit”, “TieVal”, and “JumpVal”.

The usage is

call ehsev* (SYMBOLIC-NUMBER, NEW-VALUE)

where SYMBOLIC-NUMBER is the integer number of the symbolic exceptional value from Table B.4, and NEW-VALUE is the floating point numerical value to set. So for example, to set TieVal to zero

<table>
<thead>
<tr>
<th>Symbolic Name</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>InfVal</td>
<td>1</td>
</tr>
<tr>
<td>NaNval</td>
<td>2</td>
</tr>
<tr>
<td>NoLimit</td>
<td>3</td>
</tr>
<tr>
<td>TieVal</td>
<td>4</td>
</tr>
<tr>
<td>JumpVal</td>
<td>5</td>
</tr>
</tbody>
</table>

Table B.4. Numbering of Symbolic Exceptional Values
call ehsevd(4, 0.0d0)

It is important that the numerical value be of the right type, as there is, in general, no guarantee that the compiler would convert it to the right type.

### B.6.2 Changing Exceptional Behavior for a Particular Intrinsic

To override the exceptional behavior of a particular intrinsic, one needs to know two facts: the integer that represents the intrinsic for which the exception is occurring, and the integer “offset” of the exceptional condition whose return value is to be altered. The integer representing the intrinsic can be found in Table B.5.

<table>
<thead>
<tr>
<th>Intrinsic</th>
<th>Numerical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>AINT</td>
<td>1</td>
</tr>
<tr>
<td>ANINT</td>
<td>2</td>
</tr>
<tr>
<td>DNINT</td>
<td>2</td>
</tr>
<tr>
<td>ABS</td>
<td>3</td>
</tr>
<tr>
<td>MOD</td>
<td>4</td>
</tr>
<tr>
<td>SIGN</td>
<td>5</td>
</tr>
<tr>
<td>DIM</td>
<td>6</td>
</tr>
<tr>
<td>MAX</td>
<td>7</td>
</tr>
<tr>
<td>MIN</td>
<td>8</td>
</tr>
<tr>
<td>SQRT</td>
<td>9</td>
</tr>
<tr>
<td>currently not used</td>
<td>10</td>
</tr>
<tr>
<td>currently not used</td>
<td>11</td>
</tr>
<tr>
<td>**</td>
<td>12</td>
</tr>
<tr>
<td>ASIN</td>
<td>13</td>
</tr>
<tr>
<td>ACOS</td>
<td>14</td>
</tr>
<tr>
<td>SQRT4CABS</td>
<td>15</td>
</tr>
</tbody>
</table>

Table B.5. Numbering of Intrinsic Functions

*Note:* The SQRT4CABS “function” is a dummy intrinsic generated by ADIFOR 2.0 to handle the complex ABS function. Let \( z = x + iy \). The complex \( \text{ABS}(z) \) function is rewritten as

\[
\text{abs}(z) = \text{SQRT4CABS}(x^2 + y^2)
\]

By default, SQRT4CABS has the same exceptional behavior as SQRT.

### Single Exceptional Condition

All intrinsics except for the power operator ** have only a single exceptional condition (see Tables B.2 and B.3) and therefore have an offset of one. Suppose one wishes to change the exceptional value of ABS at zero (for both real and double precision) so that the partial derivative of \( \text{ABS}(x) \) with respect to \( x \) at zero is one. First, one would look in Table B.5 to find that the integer representing \( \text{ABS} \) is 3. Hence, one would use the following two calls to set the desired partials of ABS.

```c
C Set single precision partial of abs
call ehsups (3, 1, 1.0e0)
```
xabs = abs(x)
yabs = abs(y)
w = max(xabs,yabs)
if (w .eq. 0.0) then
    z = 0.0
else
    z = w*sqrt( (xabs/w)**2 + (yabs/w)**2 )
endif

Figure B.5. Computation of Euclidean Norm with Scaling

C    Set double precision partial of abs
     call ehsupd (3,1,1.0d0)

Handling of the POWER operator (**):

As indicated in Table B.5, the integer representing the power operator is 12. The partial with respect to x is associated with an offset of 1, the partial with respect to y is associated with an offset of 2, for example:

C    Set single precision partial w.r.t. x of **
     call ehsups (12,1,1.0e0)
C    Set double precision partial w.r.t. y of **
     call ehsupd (12,2,1.0d0)

B.7 Examples of the Use of ADIntrinsics

As an example, consider the computation of the Euclidean norm \( z = \sqrt{x^2 + y^2} \). A numerically sensible way of doing this is shown in Figure B.7. This function is differentiable except for \( x = y = 0 \). However, automatically differentiating with respect to \( x \) and \( y \), we note that we might attempt to compute the derivatives of \( \text{abs()} \) when its argument is zero, and of \( \text{max()} \) when both its arguments have the same value, even when \( x \) and \( y \) are not both zero. By default, the ADIntrinsics system would invoke the error handler, which would report these exceptions to the user. However, we know that, unless \( x = y = 0 \), this computation represents a differentiable function and that, independent of the value of \( w \), we will obtain the same result.

Thus, as shown in Figure B.7, we go into “performance mode” in the part of the code that generates exceptions that are merely caused by our use of scaling, thus avoiding invocation of the error handler altogether. Also, since the value \( w \) did not have an impact on the computed value, the value for the derivative of \( w \) will not matter, either. For \( x = y = 0 \), we trigger an invocation of the ADIntrinsics error handler at the point of nondifferentiability by replacing \( z = 0 \) with \( z = \text{sqrt}(w) \). When translated by ADIFOR, the generated derivative code will report a “SQRT” exception only at \( x = y = 0 \).
C      AD_EXCEPTION_LEVEL(Performance)
      xabs = abs(x)
      yabs = abs(y)
      w = max(xabs, yabs)
C      AD_EXCEPTION_LEVEL(DEFAULT)
      if (w .eq. 0.0) then
C      the sqrt(0.0) call triggers exception reporting
      z = sqrt(w)
      else
C      AD_EXCEPTION_LEVEL(Performance)
      z = w*sqrt( (xabs/w)**2 + (yabs/w)**2 )
C      AD_EXCEPTION_LEVEL(DEFAULT)
      endif

Figure B.6. Computation of Euclidean Norm Annotated for Subsequent Automatic Differentiation
Appendix C

Sparse Derivative Support for ADIFOR 2.0 through the SparsLinC 1.1 Library

C.1 Introduction

SparsLinC 1.1 (Sparse Linear Combinations) is a library of C routines that provide an implementation of the “vector linear combination”:

$$w = \sum_{i=1}^{k} \alpha_i \cdot v_i;$$  \hspace{1cm} (C.1)

employing sparse data structures. Here $w$ and the $v_i$ are vectors, the $\alpha_i$ are scalar multipliers, and $k$ is referred to as the arity. This operation is the fundamental computational kernel for first-order automatic differentiation.

To link SparsLinC into your executable, you must add one of the following to your link line:

... -L$AD\_LIB/lib -lSparsLinC-$AD\_OS  \# in UNIX

or

... $AD\_LIB/lib/libSparsLinC-$AD\_OS.a  \# in UNIX

or

... %AD\_LIB%\lib\libSparsLinC.lib  \# in Windows-95/NT

SparsLinC utilizes dynamic data structures to represent only the nonzero information contained in each vector and performs the vector linear combinations on these sparse representations of the vectors. By doing so, it avoids storing zero values and performing computation with zeros, at the cost of introducing some overhead associated with maintaining sparse data structures.

One way of representing a sparse vector with $nnz$ nonzeros in Fortran is by means of two arrays, each of length $nnz$, one an integer array containing the indices of the nonzero entries, and the other
a floating-point array of appropriate precision, containing the corresponding values. So, for example, the 7-vector

\[(11.0, 0, 33.0, 44.0, 0, 0, 77.0)\]

would be represented by

<table>
<thead>
<tr>
<th>Index Array:</th>
<th>1</th>
<th>3</th>
<th>4</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value Array:</td>
<td>11.0</td>
<td>33.0</td>
<td>44.0</td>
<td>77.0</td>
</tr>
</tbody>
</table>

We will refer to this 2-array representation of the vector as the **Fortran Sparse Format**. The corresponding non-sparse representation, which we will call the **Fortran Nonsparse Format**, would be a floating-point array of length 7, containing zeros in entries 2, 5, and 6. Lastly, there is the **SparsLinC Sparse Format**, which is the internal SparsLinC representation of the vector.

In addition to reducing the space required to store derivative values and the time required to compute derivatives, SparsLinC is also useful for uncovering the sparsity features of a problem. For example, the detection of the sparsity pattern of Jacobians is of interest in a number of computations. The computation of the Jacobian using SparsLinC yields the sparsity pattern of the Jacobian as a natural consequence of the work it does in computing the Jacobian, and thus provides all the information needed for a sparse equation solving routine, for example. We anticipate that this feature of SparsLinC will be further strengthened in future releases with the addition of diagnostic capabilities about the “sparsity behavior” of a computation.

From the user’s point of view, using SparsLinC is very simple. Much of the task of interfacing ADIFOR 2.0-generated code and SparsLinC is done automatically and is transparent to the user. Section ?? describes how to invoke ADIFOR 2.0 to generate derivative code that uses the SparsLinC library. Such code will be referred to as “sparse derivative code.” We will refer to derivative code generated by ADIFOR 2.0 in the default case (i.e., with do-loop implementation of vector linear combinations, rather than calls to SparsLinC routines) as “nonsparse derivative code.”

Section C.2 provides some background information necessary to understand the use of SparsLinC with ADIFOR 2.0. Section C.3 defines the notion of sparsity and discusses computational scenarios where sparsity exists and can be exploited by SparsLinC for faster, less memory-intensive code. In the tutorial example given in Chapter 4, Step 4 describes, for the nonsparse (default) case, how to incorporate the ADIFOR 2.0-generated derivative code in the derivative code driver. Section C.4 outlines how this is done in the sparse derivative code driver by calling the appropriate **SparsLinC Access Routines**. These routines are the subset of SparsLinC routines that allow the user to set up and configure SparsLinC, pass data to it, and extract results and performance measures from it. Section C.5 describes how to build a sparse derivative code by using ADIFOR 2.0 and SparsLinC. Section C.6 contains detailed description of the SparsLinC access routines.

### C.2 Background

In ADIFOR 2.0, an **active variable** is one that lies on a dependency path from the independent to the dependent variables (the independents and dependents themselves are also considered to be active). Active variables are the ones for which we compute **directional derivatives** with respect to a set of (not necessarily normalized) directions specified via the seed matrix. In the simplest case, each unit direction is defined by one of the independent variables, which is equivalent to setting the seed matrix to be the identity.

We define the term **directional gradient vector** to be the set of directional derivatives of any scalar active variable with respect to all directions specified in the seed matrix. The term **scalar active variable** here refers both to active variables declared as scalars in the user’s Fortran source
code and to the individual elements of active variables that are declared as arrays. The directional gradient vectors appear as vector operands in the vector linear combinations equation (C.1).

C.3 Where Is SparsLinC Useful?

The main rationale for the development of SparsLinC is to make derivative computation run faster and use less memory. But not every problem will result in faster code if SparsLinC is used. The potential gain depends, to a large extent, on the inherent sparsity present in any particular derivative computation.

C.3.1 Definition of Sparsity

In a nonsparse representation, a directional gradient vector $V$ would be declared as an array of length $p$, where $p$ is the number of directions (i.e., the number of columns in the seed matrix). We denote the number of nonzeros in $V$ at a given point $t$ during the execution by $V_t, nnz$. The percentage of zero entries or sparsity of $V_t$ is defined as

$$V_t, sparsity := (1 - \frac{V_t, nnz}{p}) \times 100\%.$$  (C.2)

A good measure for the overall sparsity present in a derivative computation is the median of the sparsities of all directional gradient vectors during the entire execution of the derivative code.

A necessary (but not sufficient) condition for SparsLinC to improve the runtime performance of derivative computation is that the number of directions with respect to which we wish to compute derivatives be "large". This is perhaps an obvious, but nonetheless significant, point, since if the number of directions is small, directional gradient vectors will be short and any strategy to exploit sparsity will be defeated by the overhead associated with implementing that strategy. The determination of what is considered a large sparse problem is to a great extent dependent upon the nature of the problem; however, in our experience, the threshold at which our strategy becomes effective is 20–30 directions.

Another important issue concerning sparsity in derivative computations is that the sparsity of the final result (the nonzero structure of the final directional gradient vectors of the dependents) is only a lower bound on the sparsity of the intermediate directional gradient vectors; that is, the overall sparsity of the problem may be (and often is very) much higher than that of the final derivative result. In general, sparsity diminishes as the computation proceeds, because for all vector linear combinations, the nonzero index set of the resulting left-hand-side vector is the union of index sets of the right-hand-side vectors. As a consequence, in many problems, there may be a lot of "hidden" sparsity that can be exploited by using SparsLinC.

C.3.2 Sparse Derivative Problem Types

The numerical computation of gradients and Jacobians is an important step in the solution of many nonlinear problems, such as constrained optimization, mesh computations, and the solution of systems of stiff differential and algebraic equations. In many instances, these problems require deriva-

\footnote{For the sake of clarification, we note that $p$ denotes the same quantity as the Fortran variable $g, p$, used elsewhere in this document.}

\footnote{This discussion precludes the possibility of the occurrence of numerical zeros resulting from exact cancellation (e.g., $a + (-a)$) and zero multipliers. In our experience, exact cancellation rarely occurs in derivative computation, and currently, SparsLinC does not check for it (i.e., numerically zero vector entries are treated like nonzero entries). SparsLinC does, however, check for zero multipliers, and vectors with zero multipliers are not referenced.}
tive computations that have inherent sparsity. Two examples are gradients of partially separable functions and sparse Jacobians.

A function is partially separable if it can be represented as

\[ f(x) = \sum_{i=1}^{m} f_i(x), \]  

where \( m \) is the number of partitions, and where each component function, \( f_i(x) \), is typically a function of just a few of the elements of \( x \), implying that each of the corresponding directional gradient vectors, \( \nabla f_i(x) \), will be sparse, even though the aggregate \( f \) depends on all of \( x \), leading to a dense final gradient \( \nabla f(x) \). Any \( f \) with a sparse Hessian belongs to this class of problem [19], regardless of whether the partially separable structure is expressed explicitly in the code.

For many Jacobian computations, the final Jacobian is itself sparse, implying that there is much sparsity to be exploited in the intermediate computations. As discussed above, every intermediate directional gradient vector is at least as sparse as (and often much sparser than) the final Jacobian.

\section{Usage of SparsLinC Access Routines}

This section outlines the SparsLinC access routines and their use in the derivative code driver. These routines allow the user to set up and configure SparsLinC, pass data to it, and extract results and performance measures from it.

\subsection{About SparsLinC 1.1 Routines and Their Names}

SparsLinC provides multiprecision arithmetic support, meaning that the underlying vectors can be represented in \texttt{REAL}, \texttt{DOUBLE PRECISION}, \texttt{COMPLEX}, or \texttt{DOUBLE COMPLEX} precision. The routines involving a vector or vectors have a prefix letter designating the “precision” of the operation. For each precision-dependent SparsLinC routine, all instantiations of the routine have the same interface, meaning that they have the same arguments, in the same order, and with identical declarations except for the types of the vectors and multipliers (as an example, see the declaration of \texttt{VALVEC} in the definition of the \texttt{[S,D,C,Z]SPSD} routines in Section C.6).

Here is a summary of the naming conventions we have adopted for SparsLinC routines:

- The first letter will be an “\texttt{S}”, “\texttt{D}”, “\texttt{C}”, “\texttt{Z}”, or “\texttt{X}” indicating, respectively, whether the routine manipulates vectors in \texttt{REAL}, \texttt{DOUBLE PRECISION}, \texttt{COMPLEX}, or \texttt{DOUBLE COMPLEX} precision or whether it is a nonnumeric utility routine.
- The second and third letters will be “\texttt{SP}”, to denote that the routine is in the \texttt{SP}arsLin\texttt{C} library.
- The last two or three letters will be an abbreviation of the task performed by the routine.

We use the shorthand, “\texttt{[S,D,C,Z]name}” to refer to all four precision instantiations of a routine \texttt{name}.

\subsection{Declaration of Sparse Variables}

In Section C.2 we introduced the concept of directional gradient vectors. In the case of the non-sparse invocation of ADIFOR 2.0, these vectors are implemented as Fortran arrays. In the following examples in this and subsequent sections (C.4.2 - ??), assume that \( x \) is the independent variable.
(i.e., all 1000 entries of \( x \) are independent variables), \( f \) is the dependent variable, and \( w \) is an active variable we need to access in the derivative code driver:

\[
\text{REAL } x(1000), f(5), w
\]

In the nonsparse case, the derivative code generated by ADIFOR 2.0 (assuming the ADIFOR 2.0 options AD_PREFIX and AD_SEP have the default bindings of “g” and “\( _- \)”, respectively) will contain the following declarations:

\[
\text{REAL } g_x(g\_pmax\_,1000), g_f(g\_pmax\_,5), g_w(g\_pmax\_)
\]

By contrast, in the sparse case, the derivative code generated by ADIFOR 2.0 will contain the following declarations:

\[
\text{INTEGER } g_x(1000), g_f(5), g_w
\]

Note that the Fortran interface to SparsLinC declares each directional gradient vector to be an INTEGER. This is because each Fortran INTEGER gradient variable will be interpreted by SparsLinC to be a pointer to the sparse representation of the corresponding vector.

It is usually possible to clip-and-paste the declarations for the directional gradient vectors, and possibly the declarations of COMMON blocks that contain directional gradient vectors, from the code generated by ADIFOR 2.0. This is true for both nonsparse and sparse applications of ADIFOR 2.0. Just be aware that the declarations for the directional gradient vectors in the nonsparse and sparse codes are different.

Parenthetically, if you want to compare the sparse and nonsparse approaches for a particular problem, it is often good coding practice to write one driver for both, with preprocessor directives specifying the parts where the two differ. For example, for the above declaration, the following code could appear in the driver:

\[
\text{#ifdef NON SPARSE}
\text{REAL } g_x(g\_pmax\_,1000), g_f(g\_pmax\_,5), g_w(g\_pmax\_)
\text{#elif SPARSE}
\text{INTEGER } g_x(1000), g_f(5), g_w
\text{#endif}
\]

We use this format, wherever applicable (i.e., wherever corresponding sparse and nonsparse codes are present), in the rest of this discussion. (On most Unix systems, filenames ending with “.F” are interpreted by makefiles as Fortran files with preprocessor statements. Users unfamiliar with preprocessor directives can consult the “man” pages for “cpp”, the C preprocessor.)

C.4.3 Initializing and Customizing SparsLinC

SparsLinC data structures must be initialized before any computation can be performed. To this end, the user must call the routine XSPINI before all other calls to any SparsLinC (except for calls to XSPCNF, which must precede the call to XSPINI, as described below) or ADIFOR 2.0-generated routines. XSPINI takes no arguments and is called as follows:

\[
\text{CALL XSPINI}
\]

The routine XSPCNF provides a means of tuning SparsLinC data structures for a particular problem at hand. Most sparse vectors maintained by SparsLinC are stored in what is commonly referred to as the “single subscript” and “compressed subscript” scheme. The single subscript
scheme is the one already introduced in the Fortran context in Section C.1. In the compressed subscript scheme, in contrast, we keep track of nonzero index ranges. Thus the compressed subscript representation of the vector of Section C.1 would be as follows:

<table>
<thead>
<tr>
<th>Index Array:</th>
<th>1,1</th>
<th>3,4</th>
<th>7,7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value Array:</td>
<td>11.0</td>
<td>33.0</td>
<td>44.0</td>
</tr>
</tbody>
</table>

This representation is more efficient than the single-subscript representation when sparse vectors contain a good portion of contiguous nonzero index ranges. A contiguous nonzero index range is a range of indices wherein all the corresponding values are nonzeros. For example, for our vector above, the largest such range has size 2 and contains elements 3 and 4. This scenario commonly arises when computing Jacobians with banded structure or gradients of partially separable functions. SparsLinC automatically converts a vector from the single-subscript to the compressed-subscript representation when the number of nonzeros in the vector exceeds a certain threshold, called \texttt{switch\_threshold}, say.

For either representation, since the size to which vectors can grow is not known a priori, SparsLinC must provide, for the value and index arrays, a data structure capable of representing vectors of arbitrary size. The data structure currently employed in SparsLinC is a linked list of arrays each of which has a fixed number of entries. Let us denote this number of entries with \texttt{SSbucket\_size} for the single subscript scheme and \texttt{CSbucket\_size} for the compressed subscript scheme.

SparsLinC allows the user to adjust these values using the \texttt{XSPCNF} routine. For example, the sequence of calls

\begin{verbatim}
CALL XSPCNF(1,10)
CALL XSPCNF(2,500)
CALL XSPCNF(3,20)
\end{verbatim}

sets \texttt{SSbucket\_size} to 10, \texttt{CSbucket\_size} to 500, and \texttt{switch\_threshold} to 20. This would be appropriate, for example, for computing the gradient of a partially separable function (see Section C.3.2), where each $\nabla f_i$ usually contains about 20 nonzeros, and the number of independent variables is greater than 500.

While \texttt{XSPINI} assigns default values to these parameters and hence there is, from a functional perspective, no need to call \texttt{XSPCNF}, we encourage experimenting with these parameters and welcome feedback. Our experiments have shown that SparsLinC performs best if \texttt{CSbucket\_size} is close in value to the size of the largest contiguous nonzero index range present in the problem. The tradeoff is between runtime and memory, where a larger value of \texttt{CSbucket\_size} is likely to result in faster runtime, but also the dynamic allocation of more memory. In all cases, \texttt{SSbucket\_size} should be set smaller (and usually much smaller) than \texttt{CSbucket\_size} and should not exceed \texttt{switch\_threshold}. We are working on a facility to trace and assimilate SparsLinC runtime information to aid with SparsLinC performance tuning.

The user should pay heed to the following important note: \texttt{XSPCNF} may be called only before calling \texttt{XSPINI} to set \texttt{SSbucket\_size} and \texttt{CSbucket\_size}. This is because once \texttt{XSPINI} is called, the array dimensions set via these options cannot be modified. Calling \texttt{XSPCNF} to set \texttt{SSbucket\_size} and \texttt{CSbucket\_size}, after a call to \texttt{XSPINI}, will result in a runtime error. Calls to \texttt{XSPCNF} to set \texttt{switch\_threshold} can be made at any time.
C.4.4 Initializing the Seed Matrix

Each of the precision-specific SparsLinC routines [S,D,C,Z]SPSD converts a precision-specific sparse vector stored in the Fortran Sparse Format into a corresponding vector in the SparsLinC Sparse Format. In the following example, for the purpose of demonstration, we initialize columns 19 and 20 of g.x (corresponding to the derivatives of x(19) and x(20)), in both the nonsparse and sparse ways (assume that the arrays, INDVEC and VALVEC are declared appropriately):

```c
#ifndef NON_SPARSE
  g_x(7,19) = 2.0
  g_x(19,19) = 1.0
  g_x(20,20) = 1.0
#endif

else SPARSE
  INDVEC(1) = 7
  VALVEC(1) = 2.0
  INDVEC(2) = 19
  VALVEC(2) = 1.0
  CALL SSPSD(g_x(19),INDVEC,VALVEC,2)
  CALL SSPSD(g_x(20),20,1.0,1)
#endif
```

Note also that a vector must be initialized in a “one-shot” fashion; hence, for example, the following piece meal approach would be an incorrect initialization of g_x(19):

```c
INDVEC(1) = 7
VALVEC(1) = 2.0
CALL SSPSD(g_x(19),INDVEC,VALVEC,1)
INDVEC(1) = 19
VALVEC(1) = 1.0
CALL SSPSD(g_x(19),INDVEC,VALVEC,1)
```

Because of the “destructive copy” feature of SPSD (see Section C.6), the above would be equivalent to having made only the second of the two calls.

C.4.5 Extracting Directional Gradient Vectors from SparsLinC

SparsLinC provides two sets of precision-specific interfaces for extracting vector results:

```c
[S,D,C,Z]SPDXQ (XVEC, INLEN, VPTR, OUTLEN, INFO)
```

extracts sparse_object(VPTR) into the Fortran Nonspare Format vector XVEC. INLEN is the size of XVEC. The returned value OUTLEN is the largest index in the nonzero index set in sparse_object(VPTR). The value of INFO is used to indicate whether XVEC was sufficiently large to store all of the nonzero elements in sparse_object(VPTR). If OUTLEN is less than INLEN, then XVEC(OUTLEN+1:INLEN) is set to zero.

```c
[S,D,C,Z]SPXSQ (INDVEC, VALVEC, INLEN, VPTR, OUTLEN, INFO)
```

extracts sparse_object(VPTR) into the Fortran Sparse Format vector represented by the two arrays INDVEC and VALVEC. INLEN is the size of the arrays INDVEC and VALVEC. The returned value OUTLEN is the number of nonzeros in sparse_object(VPTR). The value of INFO is used to indicate whether XVEC was sufficiently large to store all of the nonzero elements in sparse_object(VPTR). If OUTLEN is less than INLEN, then VALVEC(OUTLEN+1:INLEN) and INDVEC(OUTLEN+1:INLEN) are not referenced.
In the following code segments, we show examples of the usage of these extraction routines along with the corresponding necessary declarations (there is no equivalent ADIFOR 2.0 nonsparse extraction, since in that case the output variables are already in Fortran Nonsparse Format).

**SPXDQ Example**

```fortran
PARAMETER (in_lenXd = g_pmax_)
INTEGER out_lenXd(5), infoXd(5)
REAL g_fXd(in_lenXd,5)
...
DO i = 1, 5
   CALL SSPXDQ(g_fXd(i), in_lenXd, g_f(i),
                 out_lenXd(i), infoXd(i))
ENDDO
```

**in_lenXd** is a user-defined value specifying the leading dimension of the Fortran nonsparse column vectors of **g_fXd**, i.e., it is the user’s estimate of what is the largest index corresponding to a nonzero value in the vector to be extracted. In this case, by setting **in_lenXd = g_pmax_**, we have ensured ourselves that the SparsLinC Sparse Format vector will always “fit” into the Fortran Nonsparse Format vector. (In the next example we will discuss the case of underestimating memory requirements.)

Note that as specified above, **g_fXd** is defined identically to the nonsparse **g_f** in Section C.4.2. Given Fortran’s column order array storage, the above call to **SSPXDXQ** causes **g_fXd** to be aligned exactly with the nonsparse **g_f**.

**SPXSQ Example**

```fortran
PARAMETER (in_lenXs = 40)
INTEGER g_f_indXs(in_lenXs,5), out_lenXs(5), infoXs(5)
REAL g_f_valXs(in_lenXs,5)
...
DO i = 1, 5
   CALL SSPXSQ(g_f_indXs(i), g_f_valXs(i), in_lenXs, g_f(i),
                out_lenXs(i), infoXs(i))
ENDDO
```

Here, our choice of **in_lenXs = 40** implies that we have made the assumption that there are at most 40 nonzeros in any row of the Jacobian \(\frac{\partial f}{\partial x}\) (i.e., given our declaration of \(x\) in Section C.4.2, we assume that the least sparse directional derivative vector is 96% sparse). To make sure that our memory requirement assumption holds, we add the following code:

```fortran
max_lenXs = 0
DO i = 1, 5
   IF (infoXs(i) .NE. 0 .AND. out_lenXs(i) .GT. max_lenXs) THEN
      max_lenXs = out_lenXs(i)
   END IF
END DO
```

Now **max_lenXs** is encoded with the information we need. That is, if zero, our assumption was true, else, **max_lenXs** is equal to the true number of nonzeros in the least sparse row of the Jacobian and we know how much memory is really needed to extract all nonzero derivative values.
C.4.6 Adding the Contents of a Sparse Vector to a Dense Vector

Two SparsLinC routines are provided for adding a SparsLinC Sparse Format vector to a Fortran Nonsparse Format vector.

\[ [S,D,C,Z]SPXMQ (XVEC, INLEN, MULT, V PTR, OUTLEN, INFO) \]

adds to XVEC the contents of \( \text{sparse\_object(VPTR)} \) multiplied by MULT (i.e., \( XVEC = XVEC + \text{MULT} \times \text{sparse\_object(VPTR)} \)).

\[ [S,D,C,Z]SPXAQ (XVEC, INLEN, V PTR, OUTLEN, INFO) \]

is identical to SPXMQ, except that the multiplier is assumed to be one (i.e., \( XVEC = XVEC + \text{sparse\_object(VPTR)} \)). Note that SPXMQ and SPXAQ are functionally very similar to the SPXDQ routine, the only difference being that SPXDQ "assigns to" XVEC while SPXMQ and SPXAQ "add to" XVEC the contents of the sparse vector. Note also, that the interfaces of SPXAQ and SPXDQ are identical.

C.4.7 Dumping the Contents of a Sparse Vector

SparsLinC provides a set of precision-specific interfaces for dumping a sparse vector to a file.

\[ [S,D,C,Z]SPPRQ (V PTR, EXT) \]

writes the number of nonzeros as well as index/value pairs of \( \text{sparse\_object(VPTR)} \) to stdout or a file. EXT is an INTEGER in the range \([0,999]\) and specifies the destination of the output: if zero, output is written to stdout; otherwise, output is written to the file SPPRQ.EXT.

SPPRQ can be a useful routine during debugging, to quickly check the values of a derivative vector somewhere in the code. It also has the advantage of not requiring that the user provide memory in which to extract the nonzero values in the sparse vector.

Admittedly, the interface of SPPRQ is rather crude. This is because we have avoided passing string arguments, because of the inconsistency of the Fortran-to-C string-passing protocols on different platforms.

**SPPRQ Example**

DQ i = 1, 2
    CALL SPPRQ(g_f(i), 6)
ENDDO

The above code prints the nonzero derivative information in \( g_f(1) \) and \( g_f(2) \) into the file “SPPRQ.6” in the current directory. Assume that \( g_f(1) \) and \( g_f(2) \) contain 4 and 2 nonzero values, respectively. Then the following is an example of what might be the contents of “SPPRQ.6” subsequent to the execution of the above code:

**Number of nonzeros = 4**

<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>-4.892400e+01</td>
</tr>
<tr>
<td>5</td>
<td>6.523200e+00</td>
</tr>
<tr>
<td>6</td>
<td>-1.630800e+00</td>
</tr>
<tr>
<td>188</td>
<td>-2.030000e+01</td>
</tr>
</tbody>
</table>

**Number of nonzeros = 2**
<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>3.812800e+00</td>
</tr>
<tr>
<td>256</td>
<td>1.000000e+00</td>
</tr>
</tbody>
</table>

Note that the vectors are printed out in the order in which the corresponding SPPRQ was called, and there is no identification in the file denoting which set of numbers belong to which vector. This task is left to the user.

### C.4.8 Extracting Performance Information

In addition to providing derivative information, SparsLinC can also provide information about its own performance. Because of the system-specific nature of timing routines, runtime measures, however, are best arrived at by enveloping the appropriate system calls around the call to the top level subroutine. For example:

```fortran
CALL timer(t1)
CALL g_top_foo(x, g_x, 
CALL timer(t2)
t_escaped = t2 - t1
```

The SparsLinC routine `XSPMEM` returns how many kilobytes of memory have been dynamically allocated in the process of computing derivatives:

```fortran
REAL USEDKB
...
CALL XSPMEM(USEDKB)
```

### C.4.9 Freeing Dynamically Allocated Memory

The routine `XSPFRA` frees all dynamically allocated memory in SparsLinC. Freeing memory might be useful if after finishing the derivative computation, the user wishes to perform some further memory-intensive computation. There are no arguments, and the call is simply

```fortran
CALL XSPFRA
```

`XSPFRA` has the effect of leaving “dangling pointers”, meaning that the Fortran `INTEGER` gradient variables, which are interpreted by SparsLinC as pointers, will retain the values (addresses) they contained before `XSPFRA` was called. However, after the call to `XSPFRA`, the memory pointed to by these pointers will no longer be under SparsLinC control. Any attempt to use these variables as pointers (e.g., by using them as pointer arguments to some SparsLinC routine) will likely cause a segmentation fault. For this reason, _no calls to any SparsLinC routine should be made after XSPFRA._

### C.5 A Brief Tutorial Example

SparsLinC is designed to be easy to use. First, apply ADIFOR 2.0 to generate sparse derivative code by specifying `AD_FLAVOR=sparse` in your script file. Then, create a “Sparse” derivative code driver. The derivative code driver is a user-generated Fortran program that invokes the derivative code generated by ADIFOR 2.0. In general, the sparse derivative code driver is analogous to the nonsparse derivative code driver and differs from the latter in only a few places. The following is an
example derivative code driver, based on the code fragments shown throughout Section C.4:

```c
PROGRAM DRIVER

REAL x(1000), f(5), w

#elifdef NON_SPARSE
REAL g_x(g_pmax_,1000), g_f(g_pmax_,5), g_w(g_pmax_)
#endif

#edef SPARSE
INTEGER g_x(1000), g_f(5), g_w
PARAMETER (in_len_xs = 40)
INTEGER g_f_ind_xs(in_len_xs,5), out_len_xs(5), info_xs(5)
REAL g_f_val_xs(in_len_xs,5)
REAL USEDKB
#endif

CCC We assume some statements at this point initialize the independent
CCC variables.

#edef SPARSE
CCC Tuning of SparsLinC parameters (optional) and mandatory initialization
CALL XPCNF( 1, 10 )
CALL XPCNF( 2, 500 )
CALL XPCNF( 3, 20 )
CALL XSPINI
#endif

CCC Initializing the seed matrix as identity.

#edef NON_SPARSE
DO i=1,1000
   DO j=1,1000
      g_x(i,j) = 0.0d0
   ENDDO
   g_x(i,i) = 1.0d0
ENDDO
#endif

#edef SPARSE
DO i=1,1000
   CALL SSPSD(g_x(i),i,1.d0,1)
ENDDO
#endif

#edef NON_SPARSE
   CALL g_top_foo(g_p_, x, g_x, ldg_x, f, g_f, ldg_f,
       w, g_w, ldg_w, non_active_var)
#endif

#edef SPARSE
   CALL g_top_foo(x, g_x, f, g_f, w, g_w, non_active_var)
#endif
   CALL EHRPT
#endif
```

82
DO  i = 1, 5
   CALL SSPKSQ(g_f_ind xs(i,1), g_f_val xs(i,1), in_len xs, g_f(i),
   \           out_len xs(i), info xs(i))
ENDDO
max_len xs = 0
DO i = 1, 5
   IF (info xs(i) .NE. 0 .AND. out_len xs(i) .GT. max_len xs) THEN
      max_len xs = out_len xs(i)
   ENDIF
ENDDO

CALL XSPMEM(USEDKB)
#endif

Taking a close look at the calls to the top level routine, $g_{\text{top\_foo}}$, in the driver code, we note
that the sparse call differs from the nonsparse call in that there is never a need to pass a leading
dimension argument along with each gradient variable argument, and also in that there is no need
to pass a value for $g_{\text{p\_}}$, the runtime nonsparse directional gradient vector size. Note that, regardless of
whether ADIFOR 2.0 is invoked in the sparse or nonsparse mode, it generates the same subroutine
name (assuming the ADIFOR 2.0 options \texttt{AD\_PREFIX} and \texttt{AD\_SEP} had the same bindings on both
cases).

Finally, link all the generated derivative code and your driver with the SparsLinC 1.1 as described
at the beginning of this chapter.

\section{C.6 Detailed Specification of Access Routines}

This section contains the detailed description of the SparsLinC 1.1 access routines discussed in
Section C.4.

We adopt the convention that for a Fortran INTEGER variable VPTR, acting as a pointer
to a SparsLinC Sparse Format vector, the sparse derivative object pointed to by VPTR is called
\texttt{sparse\_object(VPTR)}. Also, to save space, only the calling sequence for one particular floating-point
precision is provided.
SSPSD, DSPSD, CSPSD, ZPSD

SUBROUTINE SSPSD (VPTR, INDVEC, VALVEC, LEN)
Purpose
Conversion of a vector in Fortran Sparse Format into a vector in SparsLinC Sparse Format. The Fortran Sparse Format vector is given by the two arrays, INDVEC(1:LEN) and VALVEC(1:LEN), representing the indices and values of a sparse vector \( x \) (say), respectively. \( x \) is copied into sparse\_object(VPTR), which is the vector in SparsLinC Sparse Format. The indices in INDVEC need not be in any particular order (internally, SPSD performs an ascending order sort). However, INDVEC and VALVEC must be identically aligned. That is, if in the Fortran Nonparse Format \( x \) has a nonzero entry at index \( i \) with value \( v \), then for some \( J \), the following must hold: \( \text{INDVEC}(J) = i \) and \( \text{VALVEC}(J) = v \). SPSD performs a destructive copy. That is, if sparse\_object(VPTR) had been previously allocated (via SPSD or as a result of being an output argument of some other SparsLinC routine), the previous information in sparse\_object(VPTR) is lost, and the dynamically allocated memory where that information resided is deallocated.

Arguments

**VPTR**  
*output* INTEGER  
Upon exit, sparse\_object(VPTR) contains a copy of the sparse vector represented by INDVEC and VALVEC.

**INDVEC**  
*input* INTEGER array, dimension (LEN)  
Indices of the nonzero values of the sparse vector. (We assume that indices are \( \geq 1 \); therefore, INDVEC entries \( \leq 0 \) would be incorrect and would result in a runtime error.)

**VALVEC**  
*input* REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX] array, dimension (LEN)  
Nonzero values of the sparse vector.

**LEN**  
*input* INTEGER  
LEN \( \geq 0 \) is the number of nonzeros in the sparse vector. If LEN = 0, VPTR is initialized to point to the vector of all zeros and INDVEC and VALVEC are not referenced.

---

**SSPXDQ, DSPXDQ, CSPXDQ, ZSPXDQ**

SUBROUTINE SSPXDQ (IVEC, INLEN, VPTR, OUTLEN, INFO)

Purpose
Extracts sparse\_object(VPTR) into the Fortran Nonparse Format vector IVEC.

Arguments

**IVEC**  
*output* REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX] array, dimension (INLEN)  
On exit, if INFO = 0, IVEC(1:INLEN) will contain a dense representation of sparse\_object(VPTR). If OUTLEN < INLEN, then IVEC(OUTLEN+1:INLEN) is initialized to all zeros. If INFO \( \neq 0 \), IVEC is not referenced.

**INLEN**  
*input* INTEGER  
Length of IVEC.
VPTR
(input/output) INTEGER
Pointer to the SparseLinC Sparse Format vector. If VPTR equals NULL, it is initialized to point to the vector of all zeros (which is why it might be an output argument).

OUTLEN
(output) INTEGER
Largest index in the nonzero index set in sparse_object(VPTR). This value will always be returned, whether XVEC is initialized or not. See the description of INFO below.

INFO
(output) INTEGER
If INLEN < OUTLEN, INFO will be set to -1, and XVEC is not referenced. Otherwise, INFO is set to 0, and XVEC(1:INLEN) is initialized to a Fortran Nonsparse Format copy of sparse_object(VPTR).

SSPXSQ, DSPXSQ, CSPXSQ, ZSPXSQ

SUBROUTINE SSPXSQ (INDVEC, VALVEC, INLEN, VPTR, OUTLEN, INFO)

Purpose
Extracts sparse_object(VPTR) into the Fortran Sparse Format vector represented by the two arrays, INDVEC and VALVEC.

Arguments

INDVEC
(output) INTEGER array, dimension (INLEN)
On exit, if INFO = 0, INDVEC(1:OUTLEN) contains the indices of the nonzero entries of sparse_object(VPTR). If INFO = 0 and OUTLEN < INLEN then INDVEC(OUTLEN+1:INLEN) is not referenced. If INFO ≠ 0, INDVEC is not referenced.

VALVEC
(output) REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX] array, dimension (INLEN)
On exit, if INFO = 0, VALVEC(1:OUTLEN) will contain the nonzero entries of sparse_object(VPTR). If INFO = 0 and OUTLEN < INLEN then VALVEC(OUTLEN+1:INLEN) is not referenced. If INFO ≠ 0, VALVEC is not referenced.

INLEN
(input) INTEGER
Length of INDVEC and VALVEC.

VPTR
(input/output) INTEGER
Pointer to the SparseLinC Sparse Format vector. If VPTR equals NULL, it is initialized to point to the vector of all zeros (which is why it might be an output argument).

OUTLEN
(output) INTEGER
Number of nonzeroes in sparse_object(VPTR). This value will always be returned, whether INDVEC and VALVEC are initialized or not. See the description of INFO below.
INFO
(output) INTEGER
If INLEN < OUTLEN, INFO will be set to -1, and INVEC and VALVEC are not referenced. Otherwise, INFO is set to 0, and INVEC(1:OUTLEN) and VALVEC(1:OUTLEN) are initialized to the Fortran Sparse Format copy of sparse_object(VPTR).

SSPXMQ, DSPXMQ, CSPXMQ, ZSPXMQ

SUBROUTINE SSPXMQ (XVEC, INLEN, MULT, VPTR, OUTLEN, INFO)

Purpose
Adds the weighted contents of sparse_object(VPTR) to the Fortran Nonsparse Format vector XVEC, with MULT being the multiplicative weight (i.e., \textit{XVEC} = \textit{XVEC} + \textit{MULT} * \textit{sparse_object(VPTR)}). For example, say \textit{XVEC} is a vector of length 7 containing all ones, \textit{MULT} = 2.0, and \textit{sparse_object(VPTR)} is as follows:

| Index Array: | 1 | 3 | 4 | 7 |
| Value Array: | 11.0 | 33.0 | 44.0 | 77.0 |

Subsequent to the call to this routine, \textit{XVEC} would contain the following:

(23.0, 1.0, 67.0, 89.0, 1.0, 1.0, 155.0)

Arguments

\textbf{XVEC} (input/output) REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX]
array, dimension (INLEN)
On exit, if INFO = 0, XVEC(1:INLEN) will have added to it the weighted contributions of the values in \textit{sparse_object(VPTR)}, with MULT specifying the weight. If INFO \neq 0, \textit{XVEC} is not modified.

\textbf{INLEN} (input) INTEGER
Length of XVEC.

\textbf{MULT} (input) REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX]
Multiplier.

\textbf{VPTR} (input/output) INTEGER
Pointer to the SparsLinC Sparse Format vector. If VPTR equals NULL, it is initialized to point to the vector of all zeros (which is why it might be an output argument).

\textbf{OUTLEN} (output) INTEGER
Largest index in the nonzero index set in \textit{sparse_object(VPTR)}. This value will always be returned, whether XVEC is modified or not. See the description of INFO below.

\textbf{INFO} (output) INTEGER
If INLEN < OUTLEN, INFO will be set to -1, and XVEC is not modified. Otherwise, INFO is set to 0, and XVEC(1:INLEN) is modified as described above.
SSPXAQ, DSPXAQ, CSPXAQ, ZSPXAQ

SUBROUTINE SSPXAQ (XVEC, INLEN, VPTR, OUTLEN, INFO)

Purpose
Adds the contents of sparse\_object(VPTR) to the Fortran Nonsparse Format vector XVEC
(i.e., XVEC = XVEC + sparse\_object(VPTR)). (SPXA is identical to the SPXMQ routine with MULT = 1.0; see the documentation for SPXMQ.)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>XVEC</td>
<td>REAL</td>
<td>(input/output) REAL [DOUBLE PRECISION, COMPLEX, DOUBLE COMPLEX] array, dimension (INLEN) On exit, if INFO = 0, XVEC(1:INLEN) will have added to it the values in sparse_object(VPTR). If INFO ≠ 0, XVEC is not modified.</td>
</tr>
<tr>
<td>INLEN</td>
<td>INTEGER</td>
<td>(input) Length of XVEC.</td>
</tr>
<tr>
<td>VPTR</td>
<td>INTEGER</td>
<td>(input/output) Pointer to the SparsLinC Sparse Format vector. If VPTR equals NULL, it is initialized to point to the vector of all zeros (which is why it might be an output argument).</td>
</tr>
<tr>
<td>OUTLEN</td>
<td>INTEGER</td>
<td>(output) Largest index in the nonzero index set in sparse_object(VPTR). This value will always be returned, whether XVEC is modified or not. See the description of INFO below.</td>
</tr>
<tr>
<td>INFO</td>
<td>INTEGER</td>
<td>(output) If INLEN &lt; OUTLEN, INFO will be set to -1, and XVEC is not modified. Otherwise, INFO is set to 0, and XVEC(1:INLEN) is modified as described above.</td>
</tr>
</tbody>
</table>

SSPPRQ, DSPPRQ, CSPPRQ, ZSPPRQ

SUBROUTINE SSPPRQ (VPTR, EXT)

Purpose
Writes number of nonzeros as well as index/value pairs of sparse\_object(VPTR) onto stdout or a file, with the following format:

```
Number of nonzeros = ...

Index  Value
...
...
```

Arguments
VPTR  (input/output) INTEGER
Point to the SparsLinC Sparse Format vector. If VPTR equals NULL, it is
initialized to point to the vector of all zeros (which is why it might be an
output argument).

EXT  (input) INTEGER
Must be in the range [0,999]. If EXT = 0, output written is to stdout. Oth-
erwise EXT is converted to its ASCII equivalent and used as the extension
appended to the filename “SPKR.” and output is written to this file.

XSPCNF

SUBROUTINE XSPCNF (OPT, VAL)

Purpose
Allows user to customize SparsLinC for each run. The following table specifies for each
parameter its name, option number, default value, and range of allowable values. “SS-
bucket_size” and “CSBucket_size” are the number of entries per array in the linked list
representation of a single-subscript and compressed-subscript vector respectively. For all
vector linear combinations, if at the conclusion of the computation the left-hand-side vector
has an SS representation and the number of its nonzero entries exceeds “switch_threshold”,
the vector is converted to a CS representation.

<table>
<thead>
<tr>
<th>Name</th>
<th>OPT</th>
<th>Default</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSbucket_size</td>
<td>1</td>
<td>8</td>
<td>&gt;1</td>
</tr>
<tr>
<td>CSBucket_size</td>
<td>2</td>
<td>32</td>
<td>&gt;1</td>
</tr>
<tr>
<td>switch_threshold</td>
<td>3</td>
<td>16</td>
<td>&gt;1</td>
</tr>
</tbody>
</table>

XSPCNF with OPT = 1 or OPT = 2 may be called only before calling XSPINI. Calling
XSPCNF with OPT = 1 or 2 after a call to XSPINI will result in a runtime error. Calls to
XSPCNF with OPT = 3 can be made at any time.

Arguments

OPT  (input) INTEGER
Specifies the option number associated with a given parameter as given in
the above table.

VAL  (input) INTEGER
The new value for the parameter specified by OPT.

XSPMEM

SUBROUTINE XSPMEM (USEDKB)
Purpose

Reports how many kilobytes of memory have been allocated dynamically in SparsLinC.

Arguments

**USED** (output) REAL.
The number of kilobytes of storage allocated for SparsLinC data structures.
XSPINI

SUBROUTINE XSPINI

Purpose
Initializes the sparse data structures by dynamically allocating memory for some SparsLinC-
internal global variables. It must be called before any of the other SparsLinC routines
(except for calls to XSPCMF with OPTs 1-2) and needs to be called no more than once (when
called more than once, all but the first call act as no-ops).

Arguments
none

XSPFRA

SUBROUTINE XSPFRA

Purpose
Frees all memory allocated for C sparse vector data structures. Note: all pointers to
sparse directional gradient variables (VPR's) are left dangling.

Arguments
none
Appendix D

Installation, Configuration and Use of ADIFOR 2.0 on Windows 95/NT

D.1 Installation

D.2 Configuration

D.3 Use

The use of ADIFOR 2.0 under Windows-95/NT is practically identical to its use under Unix – you first create a composition and an ADIFOR script file, then you invoke the ADIFOR Preprocessor which is named Adifor2i passing it the same options as previously, and then you link your code against the generated derivative code and against the ADIntrinsics and SparsLinC libraries. Note that the appropriate Windows 95/NT libraries and components are named ADIntrinsics.lib, ReqADIntrinsics.obj and SparsLinC.lib.

For each of the examples that we have provided, you will find a script adANDrun.bat that can be used to invoke ADIFOR and then run the generated derivative code.
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Bibliography


