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An Introduction to Using Software Tools for Automatic Differentiation[*]

by

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Abstract

We give a gentle introduction to using various software tools for automatic differentiation (AD). Ready-to-use examples are discussed, and links to further information are presented. Our target audience includes all those who are looking for a straightforward way to get started using the available AD technology. The document is dynamic in the sense that its content will be updated as the AD software evolves.

1 Intention and References

This document explains how to use the following software tools for automatic differentiation (AD) to generate first-order derivative code for a small example problem.

- ADIFOR 2.0 Revision D (`http://www.mcs.anl.gov/adifor`)
- ADIC 1.1 (`http://www.mcs.anl.gov/adic`)
- ADOL-C 1.8 (`http://www.math.tu-dresden.de/wir/project/adolc`)
- TAPENADE 1.0-alpha (`http://www-sop.inria.fr/tropics`)

The document does not describe the AD algorithms used by these software tools. Various publications cover the theoretical foundations of the algorithms referenced in our discussion. For an introduction and more advanced issues we point the reader to [9]. Three workshops have been dedicated to AD, and the proceedings [5, 6, 7] contain numerous references to other AD-related papers that have appeared in scientific journals and proceedings of international conferences. A large variety of successful applications of AD software to real-world applications are discussed there as well.

2 Getting Started

For information on how to obtain, install, and use the AD tools discussed in this document, visit the Web sites listed in Section 1. The examples in this document are discussed in the context of the computer environment found on a laptop computer, specifically an Intel Pentium system running Mandrake Linux Version 8.1. ADIFOR, ADIC, and TAPENADE are installed in the directory `/home/uwe/ADTOOLS`. The ADOL-C library and include files are assumed to be in the same directory as the source files.

ADIFOR, ADIC, and TAPENADE are available on the Web and can be accessed online by using the corresponding Web servers. Visit

- `http://www.mcs.anl.gov/autodiff/adiforserver` for ADIFOR,
- `http://www.mcs.anl.gov/autodiff/adicserver` for ADIC, and
- `http://tapenade.inria.fr:8080/tapenade/index.jsp` for TAPENADE.

All source files presented in this document can be downloaded from

`http://www-unix.mcs.anl.gov/~naumann/ad_tools.html`.

The makefiles have to be adapted to the user's environment.

3 Explosion Equation

We have selected a variant of the Bratu problem [1] to illustrate the use of source transformation AD tools. The code in Appendix A models the thermal explosion of solid fuels, which can be described by the system of differential equations

$$x''(\tau) + s \cdot e^{\frac{x(\tau)}{1+t\cdot x(\tau)}} = 0,$$

where $\tau \in (-1, 1)$ and $x(-1) = x(1) = 0$. The problem has been discretized by using step size h as

$$F_i = x_{i-1} - 2x_i + x_{i+1} + h^2[f_{i-1} + 10f_i + f_{i+1}]/12$$

for $i = 1, \ldots, 10000$, with $x_0 = x_{10001} = 0$ and $f_i = s\exp(x_i/(1+tx_i))$. Of interest are the derivatives of the component functions F_i with respect to the current state x_i as well as the parameters s and t.

We consider the following problems:

1. ADIFOR
   - (a) Use the forward vector mode to compute the Jacobian of F with respect to x and the parameters s and t. In our implementation, F is represented by the variable `f`, x is represented by `x`, and s and t are combined into the parameter vector `prm`. All three program variables are declared as arrays of double-precision floating-point numbers, namely,
     - `double precision x(7), prm(2), f(dim)` in Fortran and
     - `double x[7], prm[2], f[7]` in C.

     (See Section 3.1.)
   - (b) Use Curtis-Powell-Reid [8] seeding to compute the compressed Jacobian in forward vector mode (see Section 3.1.1).
   - (c) Use the SparsLinC library to compute the sparse Jacobian by sparse forward mode (see Section 3.1.2).
2. ADOL-C
   - (a) Use one of the easy-to-use drivers to compute the Jacobian of F with respect to x and the parameters s and t.
   - (b) Compute the sparsity structure of the Jacobian.
   - (c) Use the low-level routines for forward and reverse mode to compute the Jacobian of F with respect to x and the parameters s and t.

   (See Section 3.3.)
3. ADIC
   - (a) Compute the Jacobian of F with respect to x in forward vector mode (see Section 3.2).
4. TAPENADE
   - (a) Compute the Jacobian of F with respect to both x and the parameters s and t in reverse mode (see Section 3.4).

3.1 ADIFOR 2.0

ADIFOR generates a differentiated version of the subroutine `expl(...)` with the following header.

```
      subroutine g_expl(g_p_, dim, parmax, x, g_x, ldg_x, prm, g_prm,
     + ldg_prm, f, g_f, ldg_f)
        integer dim, parmax
        double precision x(dim), prm(parmax)
        double precision f(dim)

        integer g_pmax_
        parameter (g_pmax_ = 9)
        integer g_p_, ldg_x, ldg_prm, ldg_f
        double precision g_x(ldg_x, dim), g_prm(ldg_prm, parmax),
     +    g_f(ldg_f, dim)
```

The parameter `g_pmax_` is the maximal number of directional derivatives that can be computed. Its value is set by using `AD_PMAX` in `explosion.adf`. The parameter is required because of the lack of dynamic memory allocation in Fortran 77. The derivative components of all scalar program variables are allocated as vectors of length `g_pmax_`. For example, in order to compute the Jacobian matrix of `f` with respect to `x`, the value of `g_pmax_` must be at least equal to 7, so that the derivative components of `x` can accommodate the identity in $I\!R^7$.

The actual number of directional derivatives `g_p_` must be less than or equal to `g_pmax_`. The parameter `g_p_` determines the upper bound for the loops that compute the values of the derivative components.

To compute the Jacobian of `f` with respect to both `x` and `prm`, we set `g_pmax_` to be greater than or equal to the sum of the numbers of elements in both vectors, that is, $9 = 7 + 2 = \text{dim} + \texttt{parmax}$. Consequently, `g_x` contains the first `dim` columns of the seed matrix and `g_prm` its last `parmax` columns. The argument `g_f` is the transpose of the (`dim` $\times$ `ldg_f`)-Jacobian, where `ldg_f` must be initialized to 9. All this is done in the driver routine, which is shown in Appendix B.3.2.

The "`dense:`" section of the makefile in Appendix B.2 builds an executable that produces the following result.

```
-1.88  1.01  0.    0.    0.    0.    0.    0.21 -0.48
 1.01 -1.87  1.01  0.    0.    0.    0.    0.39 -1.78
 0.    1.01 -1.87  1.01  0.    0.    0.    0.48 -2.69
 0.    0.    1.01 -1.87  1.01  0.    0.    0.55 -3.49
 0.    0.    0.    1.01 -1.87  1.01  0.    0.48 -2.69
 0.    0.    0.    0.    1.01 -1.87  1.01 0.39 -1.78
 0.    0.    0.    0.    0.    1.01 -1.88 0.21 -0.48
```

The output has been formatted for better readability. It shows the full 7×9 Jacobian evaluated at the argument:

```
x(1) = 1.72
x(2) = 3.45
x(3) = 4.16
x(4) = 4.87
x(5) = 4.16
x(6) = 3.45
x(7) = 1.72
```

```
prm(1) = 1.3
prm(2) = 0.245828
```

3.1.1 Compressed Jacobian – Seeding

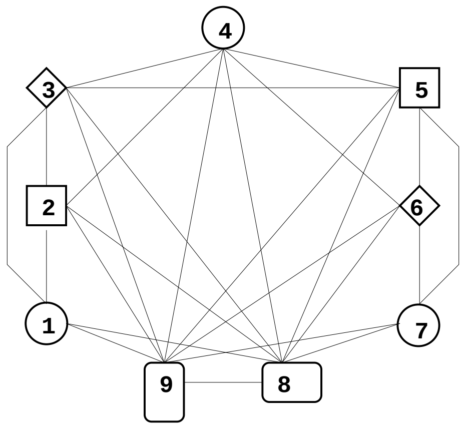
The full Jacobian computed in the preceding section is sparse, and its sparsity pattern can be visualized as follows.

$$\begin{array}{ccccccccc}
* & * & & & & & & * & * \\
* & * & * & & & & & * & * \\
 & * & * & * & & & & * & * \\
 & & * & * & * & & & * & * \\
 & & & * & * & * & & * & * \\
 & & & & * & * & * & * & * \\
 & & & & & * & * & * & *
\end{array}.$$

Here, $*$ stands for a nonzero entry, and blanks represent *structural* zero entries in the Jacobian. In other words, no dependence exists between the corresponding dependent and independent variables.

Curtis-Powell-Reid (CPR) [8] seeding is based on the idea that certain columns of the Jacobian can be merged to share storage. For example, column 1 and column 7 could share one column, thus resulting in a compressed version of the Jacobian. This implies that the sparsity pattern must be known in advance in order to exploit matrix compression techniques. Recall that the derivative code generated by ADIFOR always loops over the derivative components of all *active* variables.[‡] Many of them are equal to zero, leading to predictably trivial multiplications that one would like to avoid. Therefore, instead of computing the Jacobian as a Jacobian times identity matrix product, one could try to compute a compressed Jacobian using a seed matrix with fewer columns than the identity. Since the number of independent variables is often very large, the size of the seed matrix can become much smaller, leading to a decreased complexity of the forward vector mode Jacobian computation.

In CPR seeding, one considers the column incidence graph of the Jacobian to try to determine a minimal vertex coloring. Whenever two vertices share the same color, the corresponding columns can be stored in the same column of the compressed Jacobian. In our example, the column incidence graph has the following structure.



[‡]An active variable `w` can be characterized as follows. At some point in the program (1) the value of `w` depends on the value of some independent variables and (2) there is some dependent variable whose value depends on `w`. Variables that are not active are referred to as passive.

Unfortunately, since the vertex coloring problem is known to be NP-complete in general, the use of heuristics is essential. The coloring in the example graph has been found “by inspection.” Different colors are represented by different vertex shapes.

The number ν of different colors used determines the number of columns in the CPR seed matrix. Its rows are Cartesian basis vectors in $I\!R^{\nu}$. Whenever two vertices share the same color, the corresponding rows in the seed matrix contain the same Cartesian basis vector. This leads to the following seed matrix for our example.

$$\begin{matrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{matrix}$$

The “`compressed:`” section of the makefile in Appendix B.2 builds an executable that produces output similar to the following.

```
-1.88  1.01  0.    0.21 -0.48
 1.01 -1.87  1.01  0.39 -1.78
 1.01  1.01 -1.87  0.48 -2.69
-1.87  1.01  1.01  0.55 -3.49
 1.01 -1.87  1.01  0.48 -2.69
 1.01  1.01 -1.87  0.39 -1.78
-1.88  0.    1.01  0.21 -0.48
```

It shows the compressed 7×5 Jacobian evaluated at the current argument. The reconstruction of the original Jacobian is a simple substitution process as described in [9, Chapter 7].

3.1.2 Sparse Forward Mode – SparsLinC

We compute the Jacobian of `f` with respect to `x`. The sparsity pattern of the Jacobian need not be known a priori. Derivative components are sparse vectors of (index, value) pairs. The computational overhead of sparse vector arithmetic results from the index calculations. Structural sparsity of the extended Jacobian [9, Chapter 2] is exploited by avoiding trivial multiplications by zero. The decision about when to apply runtime sparsity methods depends on the problem structure.

The use of SparsLinC with our example can be described by the following steps:

1. Use the file `explosion.cmp` without change.
2. Add the entry `AD_FLAVOR=sparse` to `explosion.adf`.
3. Write driver program as shown in Appendix B.5.
4. Generate `g_explosion.f` by calling `Adifor2.1 AD_SCRIPT=explosion.adf`, and copy it from `output_files` to the current directory.
5. Compile `g_explosion.f` and the driver program.
6. Link with `ReqADIntrinsics-Linux86.o`, `libADIntrinsics-Linux86.a`, and `libSparsLinC-Linux86.a`.

7. Run the executable.

Let us have a closer look at the driver program. The differentiated subroutine

```
g_expl(dim,parmax,x,g_x,prm,f,g_f)
```

is generated in `g_explosion.f`, where `g_x` and `f_x` are integer arrays of dimension `dim` containing pointers to the corresponding sparse derivative objects. Seeding `g_x` is performed in the driver by

```
      do 10 i=1,dim
        g_x(i)=0
        CALL DSPSD(g_x(i),i,1.d0,1)
 10   continue
```

Notice that `g_x(i)` must be initialized properly before calling `DSPSD`. The call initializes the sparse derivative object pointed at by `g_x(i)` as (`i,1.d0`). Consequently, after executing this loop, `g_x` contains the sparse identity in $I\!R^{\mathtt{dim}}$.

The sparse derivative components are extracted by

```
      do 30 i=1,dim
        g_f(i)=0
        CALL DSPXSQ(indvec,valvec,dim,g_f(i),outlen,info)
 30   continue
```

where `indvec` is the index vector and `valvec` the corresponding value vector making up the sparse representation of the derivative object pointed at by `g_f(i)`. The parameter `outlen` is the number of nonzero entries in the `i`*th* row of the Jacobian. Consequently, the `outlen` first entries of `indvec` and `valvec` define the nonzero entries in the `i`*th* row of the Jacobian as index value pairs (`indvec(j), valvec(j)`).

The "`sparse:`" section of the makefile in Appendix B.2 builds an executable that produces output similar to the following.

```
(1, -1.88) (2,  1.01)
(1,  1.01) (2, -1.87) (3,  1.01)
(2,  1.01) (3, -1.87) (4,  1.01)
(3,  1.01) (4, -1.87) (4,  1.01)
(4,  1.01) (5, -1.87) (6,  1.01)
(5,  1.01) (6, -1.87) (7,  1.01)
(6,  1.01) (7, -1.88)
```

The sparse Jacobian is given by sparse row vectors whose nonzero entries are represented by (index, value) pairs. The reconstruction of the full Jacobian is straightforward. Refer to [3] for further information on how to use SparsLinC.

3.2 ADIC 1.1

All files involved in using ADIC with the C version of our example problem are shown in Appendix C. The Jacobian of `F` with respect to `x` is computed in forward vector mode. ADIC uses the derived data type `DERIV_TYPE` to associate derivative components with active variables. The data type `InactiveDouble` is used to indicate that some floating-point variable is not active. The call of `ad_AD_Init(dim)` causes the derivative code to use only the first `dim` elements of the derivative components. The latter are vectors of length `GRAD_MAX` (see Appendix C). The vector `x` is declared to contain the `dim` independent variables by calling

```
    ad_AD_SetIndepArray(x,dim);
    ad_AD_SetIndepDone();
```

The function value components of `DERIV_TYPE` variables are accessed by means of the macro `DERIV_val`.

ADIC generates a differentiated version of the subroutine `explosion` and names it `ad_explosion`. The argument list remains unchanged because all AD-related information is encapsulated in the new data type `DERIV_TYPE`. If the function returns a `double`, however, the differentiated function becomes a procedure, and the returned value becomes the first argument. The derivative components of scalar variables of this type can be extracted by calling the routine `ad_AD_ExtractGrad`. The actual function value can be extracted with `ad_AD_ExtractVal`. In the example we call `ad_AD_ExtractGrad(jac,F[i])` inside a loop over the `dim` elements of the vector of dependent variables `F`. The auxiliary variable `jac` is declared as a passive vector of size `dim` and contains the `i`*th* row of the Jacobian.

A makefile is provided to build the executable `explosion.ad` in order to compute the first seven columns of the Jacobian shown in Section 3.1.

3.3 ADOL-C

The AD-tool ADOL-C is based on operator overloading. Using this technique, one can log for each operation during the program execution the operator and the variables that are involved. Hence, one obtains a new internal representation of the function evaluation. Based on the generated execution log, ADOL-C computes the desired derivatives.

To apply ADOL-C for derivative calculations, one first has to modify the evaluation program to record the internal representation called tape. This modification starts with including header-file(s) that introduce the new data types and functions. Here, the easiest way is to simply include adolc.h. Second, one has to define the part of the program for which one wants to compute the derivatives. From now on, this part is called the active section. The statement trace_on(tag,*keep*); determines the beginning of the active section, the statement trace_off(*file*); the end of the active section. The parameter tag identifies the function to be differentiated. Hence, several function representations can be kept at the same time. Because of the shortness of this introduction, the optional parameters keep and file are not explained here but are explained in the documentation [4]. Third, one has to change the types of the independents to adoubles and mark them as independents using the overloaded operator <<=. Similarly, one must mark the dependents using the overloaded operator >>=. Finally, all variables that lie on the way from the independents to the dependents must be declared as adoubles. This step includes the generation of a new function explosion_ad, which contains the same source code as before but in the interface the double-variables have to be changed to adouble-variables. The required modification of the original source code is illustrated by Appendix D.

3.3.1 Jacobian Calculation with the Easy-to-Use Drivers

After the tapes are generated during the execution of the active section, the required derivative objects can be calculated. For that purpose ADOL-C provides a variety of easy-to-use drivers: gradient(..), jacobian(..), hessian(..), vec_jac(..) computing the product vector times Jacobian, jac_vec(..) computing the product Jacobian times vector, and so on. Moreover, ADOL-C supplies routines evaluating the Taylor coefficient vectors and their Jacobians with respect to the current state vector of solution curves defined by ordinary differential equations. Furthermore, there are drivers for derivative tensors and for the differentiation of implicit and inverse functions.

If one wants to compute the Jacobian of F with respect to x and the parameters s and t, one has to declare a variable storing the derivative information

```
double **J = myalloc(dim,dim+parmax);
```

where myalloc is provided by ADOL-C to allocate a two-dimensional array. Then, the statement

```
jacobian(tag,dim,dim+parmax,v,J);
```

causes the computation of the Jacobian of the function representation contained in the tape with the number tag at the point v. For a consistency check, the second and third parameter determine the number of dependents and independents, respectively. Hence, only the two statements given above have to be inserted after trace_off() in order to compute the Jacobian of F.

3.3.2 Calculation of Sparsity Pattern

ADOL-C provides for the computation of sparsity patterns the driver

```
jac_pat(tag,dim,dim+parmax,v,rb,cb,Jsp,option);
```

If one sets rb and cb to NULL, jac_pat computes the sparsity structure of the complete Jacobian at the point where the tape was generated and stores it in the unsigned int-array Jsp. The corresponding statements that have to be added to the source code are shown in Appendix D. If a certain block structure of the Jacobian is known, the unsigned int-vectors rb and cb can be applied to describe a compressed form of the independent and dependent variables.

3.3.3 Forward and Reverse Mode Using Low-Level Routines

Arbitrarily high-order derivatives can be calculated by using the low-level functions of ADOL-C for the forward and reverse mode of AD. These routines are explained in detail in a short reference available from the ADOL-C Web page. In this article, only the computation of first-order derivatives is sketched. If one wants the full Jacobian, it is preferable to use vector modes of AD. For that purpose, ADOL-C provides the drivers fov_forward(...) and fov_reverse(...). Here, fov stands for first-order vector. The other acronyms of the low-level routines have a corresponding meaning. The statement

```
fov_forward(tag,dim,dim+parmax,p,v,X,Fp,Y);
```

computes the derivative object $\mathsf{Y} = F'(v)\mathsf{X}$ for $\mathsf{X} \in I\!R^{\mathsf{dim+parmax} \times p}$. The statement

```
fov_reverse(tag,dim,dim+parmax,q,U,Z);
```

computes the derivative object $\mathsf{Z} = \mathsf{U}F'(v)$ for $\mathsf{U} \in I\!R^{q \times \mathsf{dim}}$. To prepare this reverse sweep, one has to call an appropriate forward routines, the choice of which is described in detail by the short reference mentioned above. The code segments required for computing the full Jacobian with the low-level routines are contained in Appendix D.

3.4 TAPENADE

Our last example uses the alpha version of TAPENADE 1.0 to illustrate the use of reverse-mode AD for computing the Jacobian of `f` with respect to `x` and `prm`. All files needed to run the example are described in Appendix E. The makefile in Appendix E.1 can be used to generate the executable `explosion.ad`. Running the latter results in the computation of the full Jacobian as in Section 3.1 but this time using the reverse mode of AD.

The following command-line parameters are used to call `tapenade`:

- "`-head`": The name of the head routine
- "`-vars`": The names of the independent variables
- "`-cl`": Switch indicating that reverse, or cotangent linear, mode is used

It generates derivative code in `explcl.f`, which must be compiled together with the driver program shown in Appendix E.2 and linked with the routines for storing and restoring the values of the tape as described in [9, Chapter 2].

The current version of TAPENADE does not provide the reverse vector mode. Hence, the Jacobian must be computed as a sequence of Jacobian transposed times vector products. This computation is done in the driver program by successively initializing the derivative components `g_f` of `f` as the Cartesian basis vectors in $\mathbb{R}^{\texttt{dim}}$. Thus, the Jacobian is accumulated row by row at a computational complexity proportional to the number of dependent variables. This feature becomes particularly interesting in the case of large, single gradients. Refer to [9] for further details on reverse-mode AD.

A Original Code

```
      subroutine bratu(dim,parmax,x,prm,F)
      integer    dim    , parmax
C     independent variables
      double precision x(dim), prm(parmax)
C     dependent variables
      double precision F(dim)
C
      integer i
      double precision h

      h = 2.0/(dim+1)
      F(1) = -2*x(1)+h*h*prm(1)/12.0*(1+10*exp(x(1)/(1.0+prm(2)*x(1))))
      F(2) = x(1)+h*h*prm(1)/12.0*exp(x(1)/(1.0+prm(2)*x(1)))

      do 1 i=2,dim-1
        F(i-1) = F(i-1)+x(i)+h*h*prm(1)/12.0*exp(x(i)/(1.0+prm(2)*x(i)))
        F(i) = F(i)-2*x(i)+h*h*prm(1)/1.2*exp(x(i)/(1.0+prm(2)*x(i)))
        F(i+1) = x(i)+h*h*prm(1)/12.0*exp(x(i)/(1.0+prm(2)*x(i)))
    1 continue

      F(dim-1) = F(dim-1)+x(dim)+h*h*prm(1)/12.0*exp(x(dim)/(1.0
     *           +prm(2)*x(dim)))
     F(dim) = F(dim)-2*x(dim)
     F(dim) = F(dim)+h*h*prm(1)/12.0*(1+10*exp(x(dim)/(1.0
     *         +prm(2)*x(dim))))
      end
```

B ADIFOR 2.0

The following files can be downloaded from

`http://www-unix.mcs.anl.gov/˜naumann/ad_tools.html`

```
explosion.adf
explosion.cmp
explosion.driver.compressed.f
explosion.driver.f
explosion.driver.sparse.f
explosion.f
explosion.sparse.adf
makefile
```

B.1 explosion.cmp

The composition file lists the names of all files containing subroutines subject to differentiation. In our simple example there is just `explosion.f`.

B.2 makefile

The `makefile` can be used for computing the full, compressed, and sparse Jacobians using ADIFOR 2.0. It also ensures a proper cleanup of all files that are generated automatically during this process.

```
AD_LIB=/home/uwe/ADTOOLS/ADIFOR2/ADIFOR2.0D.lib

dense:
Adifor2.1 AD_SCRIPT=explosion.adf
cp output_files/g_explosion.f .
g77 -g -c g_explosion.f explosion.driver.f
g77 -g -o explosion.ad.dense -L$(AD_LIB)/lib *.o \
$(AD_LIB)/lib/ReqADIntrinsics-Linux86.o \
-lADIntrinsics-Linux86

compressed:
Adifor2.1 AD_SCRIPT=explosion.adf
cp output_files/g_explosion.f .
g77 -g -c g_explosion.f explosion.driver.compressed.f
g77 -g -o explosion.ad.compressed -L$(AD_LIB)/lib *.o \
$(AD_LIB)/lib/ReqADIntrinsics-Linux86.o \
-lADIntrinsics-Linux86

sparse:
Adifor2.1 AD_SCRIPT=explosion.sparse.adf
cp output_files/g_explosion.f .
g77 -g -c g_explosion.f explosion.driver.sparse.f
g77 -g -o explosion.ad.sparse -L$(AD_LIB)/lib *.o \
$(AD_LIB)/lib/ReqADIntrinsics-Linux86.o \
-lADIntrinsics-Linux86 \
-lSparsLinC-Linux86

clean:
rm -fr output_files
rm -fr AD_cache
rm *.o
rm g_*
rm explosion.ad.*
rm *\~
```

B.3 Jacobian

B.3.1 explosion.adf

The Jacobian of the output variable `f` with respect to the two input variables `x` and `prm` of the top-level routine `expl` is computed. The parameter `AD_PMAX` must be set to the total number of independent variables, that is, 9[§].

```
AD_PROG = explosion.cmp
```

[§]This is because the Jacobian is computed by forward vector mode with a seed matrix that is equal to the identity in $\mathbb{R}^9$.

```
AD_TOP  = expl
AD_PMAX = 9
AD_IVARS= x prm
AD_DVARS= f
```

B.3.2 explosion.driver.f

```
      program main
      implicit none
C
C     Example: Explosion Equation
C     Driver for computing Jacobian
C
      integer dim, parmax, n
      parameter (dim=7, parmax=2, n=9)
      integer i,j
C     independent variables
      double precision x(dim), prm(parmax)
C     derivative components of independent variables
      double precision g_x(n,dim)
      double precision g_prm(n,parmax)
C     dependent variables
      double precision f(dim)
C     derivative components of dependent variables
      double precision g_f(n,dim)

C     Initialization of input variables
      x(1) = 1.72
      x(2) = 3.45
      x(3) = 4.16
      x(4) = 4.87
      x(5) = 4.16
      x(6) = 3.45
      x(7) = 1.72
      prm(1) = 1.3
      prm(2) = 0.245828

C     Seeding (identity)
      do 20 i=1,n
        do 10 j=1,parmax
          if (i.eq.j+dim) then
            g_prm(i,j)=1.0
          else
            g_prm(i,j)=0.0
          endif
 10     continue
 20   continue

      do 40 i=1,n
        do 30 j=1,dim
          if (i.eq.j) then
```

```
            g_x(i,j)=1.0
          else
            g_x(i,j)=0.0
          endif
 30     continue
 40   continue

C     call differentiated subroutine
      call g_expl(n,dim,parmax,x,g_x,n,prm,g_prm,n,f,g_f,n);

C     print Jacobian
      do 60 i=1,dim
        do 50 j=1,n
          print*, "f'(", i, ",", j, ")=",g_f(j,i)
 50     continue
 60   continue

      end
```

B.4 Compressed Jacobian

B.4.1 explosion.adf

This is the same as in the dense case.

B.4.2 explosion.driver.compressed.f

```
      program main
      implicit none
C
C     Example: Explosion Equation
C     Driver for computing compressed Jacobian
C
      integer dim, parmax, n
      parameter (dim=7, parmax=2, n=5)
      integer i,j
C     independent variables
      double precision x(dim), prm(parmax)
C     derivative components of independent variables
      double precision g_x(n,dim)
      double precision g_prm(n,parmax)
C     dependent variables
      double precision f(dim)
C     derivative components of dependent variables
      double precision g_f(n,dim)

C     Initialization of input variables
      x(1) = 1.72
      x(2) = 3.45
      x(3) = 4.16
      x(4) = 4.87
      x(5) = 4.16
      x(6) = 3.45
      x(7) = 1.72
      prm(1) = 1.3
      prm(2) = 0.245828

C     Seeding (CPR)
      do 20 i=1,n
        do 10 j=1,parmax
          g_prm(i,j)=0.0
 10     continue
 20   continue

      g_prm(n-1,1)=1.0
      g_prm(n,2)=1.0

      do 40 i=1,n
        do 30 j=1,dim
          g_x(i,j)=0.0
 30     continue
 40   continue

      g_x(1,1)=1.0
      g_x(1,4)=1.0
      g_x(1,7)=1.0
      g_x(2,2)=1.0
      g_x(2,5)=1.0
      g_x(3,3)=1.0
      g_x(3,6)=1.0

C     call differentiated subroutine
      call g_expl(n,dim,parmax,x,g_x,n,prm,g_prm,n,f,g_f,n);

C     print compressed Jacobian
      do 60 i=1,dim
        do 50 j=1,n
          print*, "f'(", i, ",", j, ")=",g_f(j,i)
 50     continue
 60   continue

      end
```

B.5 Sparse Jacobian

B.5.1 explosion.sparse.adf

In order to make ADIFOR generate derivative code that can use the sparse forward mode provided by SparsLinC, the parameter `AD_FLAVOR` must be set to `sparse`.

```
AD_PROG = explosion.cmp
AD_FLAVOR = sparse
AD_TOP  = expl
AD_PMAX = 9
```

```
AD_IVARS= x
AD_DVARS= f
```

B.5.2 explosion.driver.sparse.f

```
      program main
      implicit none
C
C     Example: Explosion Equation
C     Driver for computing sparse Jacobian using SparsLinC
C
      integer dim, parmax, n
      parameter (dim=7, parmax=2, n=9)
      integer i,j
C     independent variables
      double precision x(dim)
C     passive inputs
      double precision prm(parmax)
C     pointers to sparse derivative components of
C     independent variables
      integer g_x(dim)
C     dependent variables
      double precision f(dim)
C     pointers to sparse derivative components of
C     dependent variables
      integer g_f(dim)

C     (index, value) pairs
      integer indexes(dim)
      double precision values(dim)

C     values used in extraction routine
      integer outlen, info



C     Initialization of input variables
      x(1) = 1.72
      x(2) = 3.45
      x(3) = 4.16
      x(4) = 4.87
      x(5) = 4.16
      x(6) = 3.45
      x(7) = 1.72
      prm(1) = 1.3
      prm(2) = 0.245828

C     Initialization of sparse data structures
      call XSPINI
```

```
C     Seeding (sparse identity)
      do 10 i=1,dim
        g_x(i)=0
        g_f(i)=0
        call DSPSD(g_x(i),i,1.d0,1)
 10   continue

C     Call differentiated subroutine

      call g_expl(dim,parmax,x,g_x,prm,f,g_f)

C     Extract derivative components
      do 30 i=1,dim
        call DSPXSQ(indexes,values,dim,g_f(i),outlen,info)
        if (info.eq.0) then
          do 20 j=1,outlen
            print*, "indexes(", i, ",", j, ")=", indexes(j)
            print*, "values(", i, ",", j, ")=", values(j)
 20       continue
        endif
 30   continue

      end
```

C ADIC 1.1

The following files can be downloaded from

`http://www-unix.mcs.anl.gov/~naumann/ad_tools.html`

```
explosion.c
explosion.driver.c
explosion.init
makefile
```

C.1 makefile

```
AD_INC = -I$(ADIC)/include -I.
AD_LIB = -L$(ADIC)/lib/$(ADIC_ARCH)

all:
adiC -d gradient -i explosion.init
g++ -g -o explosion.ad $(AD_INC) $(AD_LIB) \
explosion.ad.c explosion.driver.c \
-lADIntrinsics-C -laif_grad -lm

clean:
rm explosion.ad*
rm ad_deriv.h
rm *\~
```

The environment variable `ADIC` must be set to the directory in which ADIC has been installed.

C.2 explosion.init

```
[SOURCE_FILES]
  explosion.c

[gradient]
  GRAD_MAX=7
```

The script file specifies the input files (only one in this case) and a variety of other parameters that can be looked up in [2]. The definition of GRAD_MAX, the length of the derivative components, is important. Its default value is 5, which would cause trouble in our case where dim=7 > 5. Refer to [2] for other ways to set the value of GRAD_MAX.

C.3 explosion.driver.c

```
#include "ad_deriv.h"
#include <stdio.h>
#include <iostream>
#include <stdlib.h>

extern void ad_explosion(int, DERIV_TYPE*, DERIV_TYPE*, DERIV_TYPE*);

void main()
{
  int i,j;
  int dim=7;
  int parmax=2;
  // independent variables
  DERIV_TYPE *x = new DERIV_TYPE[dim];
  DERIV_TYPE *prm = new DERIV_TYPE[parmax];
  // independent variables
  DERIV_TYPE *F = new DERIV_TYPE[dim];
  // independent variables
  InactiveDouble *jac = new InactiveDouble[dim];

  ad_AD_Init(dim);

  ad_AD_SetIndepArray(x,dim);
  ad_AD_SetIndepDone();

  DERIV_val(x[0]) = 1.72;
  DERIV_val(x[1]) = 3.45;
  DERIV_val(x[2]) = 4.16;
  DERIV_val(x[3]) = 4.87;
  DERIV_val(x[4]) = 4.16;
  DERIV_val(x[5]) = 3.45;
  DERIV_val(x[6]) = 1.72;
  DERIV_val(prm[0]) = 1.3;
  DERIV_val(prm[1]) = 0.245828;

  ad_explosion(dim,x,prm,F);
  for (i=0;i<dim;i++) {
    ad_AD_ExtractGrad(jac,F[i]);
    for (j=0;j<dim;j++)
      cout << "f'[" << i+1 << "," << j+1 << "]=" << jac[j] << endl;
  }

  ad_AD_Final();
}
```

D ADOL-C

D.1 Modifications of Original Source Code

```
#include <adolc.h>
#include <SPARSE/sparse.h>
#include <stdio.h>
#include <iostream>
#include <stdlib.h>

extern void explosion_ad(int, adouble*, adouble*, adouble*);

void main()
{
  int i,j;
  int dim=7;
  int parmax=2;
  int tag = 1;


  // independent variables (passiv)
  double *v = new double[dim+parmax];
  // dependent variables (passiv)
  double *Fp = new double[dim];


  // independent variables (active)
  adouble *x = new adouble[dim];
  adouble *prm = new adouble[parmax];
  // dependent variables (active)
  adouble *F = new adouble[dim];


  v[0] = 1.72;
  v[1] = 3.45;
  v[2] = 4.16;
  v[3] = 4.87;
  v[4] = 4.16;
  v[5] = 3.45;
  v[6] = 1.72;
  v[7] = 1.3;
  v[8] = 0.245828;
  trace_on(tag);
    for(j=0;j<dim;j++)
      x[j] <<= v[j];
    for(j=0;j<parmax;j++)
      prm[j] <<= v[j];

    explosion_ad(dim,x,prm,F);

    for(j=0;j<dim;j++)
      F[j] >>= Fp[j];
  trace_off();

}
```

D.2 Computation of Sparsity Pattern

```
  // Sparsity pattern declarations
  int option[3];
  unsigned int** Jsp = new unsigned int*[dim];

  for(j=0;j<dim;j++)
    Jsp[j] = new unsigned int[dim+parmax];
  option[0] = 0; // automatic detection for AD mode
  option[1] = 0; // save propagation of bit-pattern
  option[2] = 0; // no output

  ...

  // Sparsety pattern computation after trace_off

  jac_pat(tag,dim,dim+parmax,v,NULL,NULL,Jsp,option);
```

D.3 Jacobian Calculation Using Low-Level Routines

```
  // Calculate Jacobian using forward mode driver
  double** X = myalloc(dim+parmax,dim+parmax);
  // Calculate Jacobian using reverse mode driver
  double** U = myalloc(dim,dim);

  ...

  // Use low level routines to compute Jacobian
  // forward:

  for (j=0;j<dim+parmax;j++)
  {
   for (i=0;i<dim+parmax;i++)
     X[j][i] = 0.0;
   X[j][j] = 1.0;
  }

  // first order vector mode forward
  // ^     ^     ^            ^^^^^^^ = fov_forward
  fov_forward(tag,dim,dim+parmax,dim+parmax,v,X,Fp,J);

  // reverse
  for (j=0;j<dim;j++)
  {
   for (i=0;i<dim;i++)
     U[j][i] = 0.0;
   U[j][j] = 1.0;
  }

  // prepare reverse sweep with appropriate forward sweep
  zos_forward(tag,dim,dim+parmax,1,v,Fp);

  // first order vector mode reverse
  // ^     ^     ^            ^^^^^^^ = fov_reverse
  fov_reverse(tag,dim,dim+parmax,dim,U,J);
```

E TAPENADE

The following files can be downloaded from

http://www-unix.mcs.anl.gov/˜naumann/ad_tools.html

```
explosion.f
explosion.driver.f
makefile
```

E.1 makefile

```
ADSTACK = $(HOME)/ADTOOLS/TAPENADE/tapenade1.0/stack/adStack.o

all:
tapenade -head expl -vars "x prm" -cl explosion.f
g77 -o explosion.ad explcl.f explosion.driver.f \
$(ADSTACK)

clean:
rm explosion.ad
rm explcl.f
rm -fr diffgen
rm *\~
```

E.2 explosion.driver.f

```
      program main
      implicit none
```

```
C
C     Example: Explosion Equation
C
C     Driver for computing Jacobian using TAPENADE's
C     Reverse Mode
C

      integer dim, parmax, n
      parameter (dim=7, parmax=2, n=9)
      integer i,j
C     independent variables
      double precision x(dim), prm(parmax)
C     derivative components of independent variables
      double precision g_x(dim)
      double precision g_prm(parmax)
C     dependent variables
      double precision f(dim)
C     derivative components of dependent variables
      double precision g_f(dim)
C     the whole Jacobian matrix
      double precision jac(dim,n)

C     Initialization of input variables
      x(1) = 1.72
      x(2) = 3.45
      x(3) = 4.16
      x(4) = 4.87
      x(5) = 4.16
      x(6) = 3.45
      x(7) = 1.72

      prm(1) = 1.3
      prm(2) = 0.245828

C     Compute Jacobian as sequence of Jacobian transposed
C     times vector products
      do 40 i=1,dim
        do 10 j=1,dim
          g_f(j)=0.d0
          g_x(j)=0.d0
 10     continue
        g_f(i)=1.d0
        g_prm(1)=0.d0
        g_prm(2)=0.d0
        call explcl(dim,parmax,x,g_x,prm,g_prm,f,g_f);
        do 20 j=1,dim
          jac(i,j)=g_x(j)
 20     continue
        do 30 j=1,parmax
          jac(i,j+dim)=g_prm(j)
 30     continue
 40   continue

C     print Jacobian
      do 60 i=1,dim
        do 50 j=1,n
          print*, "f'(", i, ",", j, ")=",jac(i,j)
 50     continue
 60   continue

      end
```

References

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[3] C. Bischof, A. Carle, P. Hovland, P. Khademi, and A. Mauer, *ADIFOR 2.0 User's Guide (Revision D)*, Argonne Technical Memorandum ANL/MCS-TM-192, Argonne National Laboratory, Mathematics and Computer Science Division, 1998.

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