Extending Compile-Time Reverse Mode and Exploiting Partial Separability in ADIFOR

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by

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Abstract. The numerical methods employed in the solution of many scientific computing problems require the computation of the gradient of a function $f : \mathbf{R}^n \rightarrow \mathbf{R}$. ADIFOR is a source translator that, given a collection of subroutines to compute f, generates Fortran 77 code for computing the derivative of this function. Using the so-called torsion problem from the MINPACK-2 test collection as an example, this paper explores two issues in automatic differentiation: the efficient computation of derivatives for partial separable functions and the use of the compile-time reverse mode for the generation of derivatives. We show that orders of magnitudes of improvement are possible when exploiting partial separability and maximizing use of the reverse mode.

1 Introduction

Differentiation is one of the most fundamental mathematical concepts. In system analysis and control, the investigation into the effect of a disturbance or a change in design parameters on the performance of the overall system is essential. Mathematically, the change can be modeled by the derivative of the system output with respect to a design parameter. Another application is the numerical solution of initial value problems in stiff ordinary differential equations (see, for example [7, 18]). Methods such as implicit Runge-Kutta and backward differentiation formula (BDF) methods require a Jacobian which is either supplied by the user or approximated by finite differences. In the context of optimization, one needs the derivatives of the objective function. For example, given a function

$$f : \mathbf{R}^n \rightarrow \mathbf{R},$$

one can find a minimizer x_* of f using variable metric methods that involve the iteration

```
for $i = 1, 2, ....$ do
    Solve $B_i s_i = -\nabla f(x_i)$
    $x_{i+1} = x_i + \alpha_i s_i$
end for
```

where B_i is a symmetric positive definite matrix approximating the Hessian of f at x_i.

These methods are examples of typical methods applied in numerical computations, where the computation of the derivative is a crucial step in the numerical solution process ([6, 9, 12, 8, 21]). One particular optimization problem is the elastic plastic torsion problem, which arises from the determination of the stress field on an infinitely long cylindrical bar. The infinite-dimensional version of this problem is of the form

$$\min\{g(v) : v \in K\},$$

where $q : K \to R$ is the quadratic

$$q(v) = \frac{1}{2}\int_D \| \nabla v(x)\|^2 dx - c\int_D v(x)dx$$

for some constant c, and D is a bounded domain with smooth boundary. The convex set K is defined by

$$K = \{v \in H_0^1(D) : | v(x) | \leq dist(x, \partial D), x \in D\},$$

where $dist(x, \partial D)$ is the distance function to the boundary of D, and $H_0^1(D)$ is the Hilbert space of all functions with compact support in D such that v and $\| \nabla v\|^2$ belong to $L^2(D)$. This formulation and the physical interpretation of the torsion problem are discussed in the test problem collection of MINPACK-2 [1]. A finite element approximation of the torsion problem leads to

$$q(v) = \frac{1}{2}\sum q_{i,j}^L(v) + \frac{1}{2}\sum q_{i,j}^U(v) - h_x h_y \sum w_l(z_{i,j})v_{i,j},$$

where

$$q_{i,j}^L(v) = \mu_{i,j}\left\{ \left(\frac{v_{i+1,j}-v_{i,j}}{h_{hx}} \right)^2 + \left(\frac{v_{i,j+1}-v_{i,j}}{h_{hy}} \right)^2 \right\},$$

$$q_{i,j}^U(v) = \lambda_{i,j}\left\{ \left(\frac{v_{i-1,j}-v_{i,j}}{h_{hx}} \right)^2 + \left(\frac{v_{i,j-1}-v_{i,j}}{h_{hy}} \right)^2 \right\},$$

and $\mu_{i,j}$, $\lambda_{i,j}$, h_x, and h_y are constants.

Note that $q_{i,j}^L(v)$ and $q_{i,j}^U(v)$ are quadratics which depend only on $v_{i+1,j}$, $v_{i,j+1}$, $v_{i,j}$, and on $v_{i-1,j}$, $v_{i,j-1}$, $v_{i,j}$, respectively. The third contribution to $q(v)$, which is the linear part, depends only on $v_{i,j}$. So if we define

$$S_1 = \sum q_{i,j}^L(v)$$
$$S_2 = \sum q_{i,j}^U(v)$$
$$S_3 = \sum w_l(z_{i,j})v_{i,j},$$

then

$$f(x) = \frac{1}{2}S_1 + \frac{1}{2}S_2 - h_x h_y S_3.$$

In the MINPACK-2 code for the torsion problem shown in Appendix A, LOOP1, LOOP2, and LOOP3 correspond to the computation of S_1, S_2, and S_3, respectively.

The torsion problem is a particular instance of a particular class of functions that arises often in optimization contexts, the so-called partially separable functions [11,17,19]. These are functions $f : \mathbf{R}^n \to \mathbf{R}$ which can be expressed as

$$f(x) = \sum_{i=1}^{nb} \alpha_i f_i(x).$$

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.

ADIFOR (Automatic Differentiation of Fortran) is a source translator that augments Fortran codes with statements for the computation of derivatives [3, 2]. ADIFOR employs a mixed forward/reverse mode paradigm. The forward mode propagates derivatives of intermediate variables with respect to the input variables; the reverse mode propagates derivatives of the final values with respect to intermediate variables [14]. The forward mode follows the flow of execution of the original program, whereas the reverse mode of automatic differentiation requires the ability to access values generated in the execution of a program *in reverse order*, which is usually achieved by logging all values on a so-called *tape*, and then interpreting the tape in reverse order [14, 16, 15]. ADIFOR pioneered the use of the compile-time reverse mode where, instead of logging values at run time, we apply the reverse mode at *compile time*, thereby eliminating the storage requirements and run-time overhead of the tape scheme.

In this paper, we are concerned with the efficient generation of derivative code through the reverse mode of automatic differentiation, and the efficient use of the generated derivative code for computing gradients of partially separable functions. We use the torsion problem as a case study and explore how to improve the current ADIFOR-generated code and decrease the time and storage complexity of computing derivatives.

The paper is structured as follows. In the next section, we recall the key points about the method that is currently used in ADIFOR to generate derivatives. In Section 3, we then illustrate extensions of the compile-time reverse mode from basic blocks all the way to generating an adjoint code for the whole program. In Section 4, we explore the use of partial separability in computing derivatives. We present experimental results on Sparc-2 and IBM RS6000/550 workstations in Section 5.

2 Current ADIFOR Strategy

Automatic differentiation techniques rely on the fact that every function, no matter how complicated, is executed on a computer as a (potentially very long) sequence of elementary operations such as additions, multiplications, and elementary functions such as sin and cos. By applying the chain rule

$$\frac{\partial}{\partial t} f(g(t))|_{t=t_0} = \left(\frac{\partial}{\partial s} f(s)|_{s=g(t_0)}\right) \left(\frac{\partial}{\partial t} g(t)|_{t=t_0}\right) \tag{1}$$

over and over again to the composition of those elementary operations, one can compute derivative information of f exactly and in a completely mechanical fashion [5]. ADIFOR transforms Fortran 77 programs using this approach.

To illustrate automatic differentiation with current ADIFOR, we differentiate the subroutine `torfcn` for the torsion problem that maps an n-vector `x` into a scalar `f`. The vector `x` contains the independent variables, and the scalar `f` contains the dependent variable. The full code for `torfcn` can be found in the appendix.

The first loop (LOOP1) is shown in Figure 1. It computes S_1, whose value is stored in `fquad`. Currently, ADIFOR generates the code shown in Figure 2 for computing $\frac{\mathtt{dfquad}}{\mathtt{dx}}$. In accordance

```
      fquad = 0.0
      do 20 j = 0, ny
         do 10 i = 0, nx
            k = nx*(j-1) + i
            vr = 0.0
            vu = 0.0
            if (i .ge. 1 .and. j .ge. 1) v = x(k)
            if (i .lt. nx .and. j .gt. 0) vr = x(k+1)
            if (i .gt. 0 .and. j .lt. ny) vu = x(k+nx)
            fquad=fquad + hyx*(vr-v)**2 + hxy*(vu-v)**2
 10         continue
 20      continue
```

Figure 1: Code for LOOP1

with the specification of ADIFOR (see [3]), **g$p** denotes the actual length of the derivative objects in a call to derivative code. Since Fortran 77 does not allow dynamic memory allocation, derivative objects for local variables are statically allocated with leading dimension **pmax**. **pmax** is specified by the user when ADIFOR processes the Fortran code for **torfcn**. A variable and its associated objects are treated in analogous manner; that is, if **x** is function parameter, so is **g$x**. Derivative objects corresponding to locally declared variables or variables in common blocks are declared as local variables or variables in common blocks. Given **x** and **g$x**, the derivative code computes

$$\mathbf{g\$fquad}(1:\mathbf{g\$p}) = \left(\left(\frac{d\mathbf{fquad}}{d\mathbf{x}} \right) \mathbf{g\$x}(1:\mathbf{g\$p}, 1:\mathbf{n})^T \right)^T .$$

In particular, if **g$p** equals n and **g$x** is the $n \times n$ identity matrix, it computes the gradient of **fquad** with respect to **x**.

An active variable is one that is on the computational path from independent to dependent variables (see [4]). Notice that in the ADIFOR-generated code, a loop of length **g$p** is associated with every assignment statement involving an active variable. Therefore the cost of floating-point operations can be approximated as ($g\$p \times$ *function evaluation*). The storage requirement for ADIFOR-generated code is ($g\$p \times$ *number of active variables*). We note two key points about the current ADIFOR:

- ADIFOR uses the forward mode overall to compute derivatives. That is, ADIFOR code maintains the derivatives of intermediate variables with respect to all input variables. So, for example, **g$vu**= $\frac{d\mathbf{vu}}{d\mathbf{x}}$.
- ADIFOR uses the reverse mode to preaccumulate "local" derivatives for assignments statements.

The reverse mode is best understood with an example. For example, in the torsion problem, we have the assignment

$$\mathbf{fquad} = \mathbf{hyx} * (\mathbf{vr} - \mathbf{v}) * *2 + \mathbf{hxy} * (\mathbf{vu} - \mathbf{v}) * *2,$$

```
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
          G$FQUAD(G$I$) = 0.0d0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              DO G$I$ = 1,G$P$
                  G$V(G$I$) = 0.0d0
              END DO
              VR = 0.0
              DO G$I$ = 1,G$P$
                  G$VR(G$I$) = 0.0d0
              END DO
              VU = 0.0
              DO G$I$ = 1,G$P$
                  G$VU(G$I$) = 0.0d0
              END DO
              IF (I.GE.1 .AND. J.GE.1) THEN
C                   v = x(k)
                  DO G$I$ = 1,G$P$
                      G$V(G$I$) = G$X(G$I$,K)
                  END DO
                  V = X(K)
              END IF
              IF (I.LT.NX .AND. J.GT.0) THEN
C                    vr = x(k + 1)
                  DO G$I$ = 1,G$P$
                      G$VR(G$I$) = G$X(G$I$,K+1)
                  END DO
                  VR = X(K+1)
              END IF
              IF (I.GT.0 .AND. J.LT.NY) THEN
C                   vu = x(k + nx)
                  DO G$I$ = 1,G$P$
                      G$VU(G$I$) = G$X(G$I$,K+NX)
                  END DO
                  VU = X(K+NX)
              END IF
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
              D$0 = VR - V
              D$4 = VU - V
              DO G$I$ = 1,G$P$
                  G$FQUAD(G$I$) = G$FQUAD(G$I$) + HYX*2*D$0*G$VR(G$I$) +
     +                            (- (HXY*2*D$4)- (HYX*2*D$0))*
     +                            G$V(G$I$) + HXY*2*D$4*G$VU(G$I$)
              END DO
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
   10         CONTINUE
99999     CONTINUE
   20     CONTINUE
99998 CONTINUE
```

Figure 2: ADIFOR-generated Derivative Code for LOOP1

where $\mathtt{hxy}$ and $\mathtt{hyx}$ are constants. The chain rule tells us that

$$\nabla \mathtt{fquad} = \frac{\partial\, \mathtt{fquad}}{\partial\, \mathtt{vr}} * \nabla \mathtt{vr} + \frac{\partial\, \mathtt{fquad}}{\partial\, \mathtt{vu}} * \nabla \mathtt{vu} + \frac{\partial\, \mathtt{fquad}}{\partial\, \mathtt{v}} * \nabla \mathtt{v}.$$

Hence, if we know the "local" derivatives $(\frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{v}}, \frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{vu}}, \frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{vr}})$ of **fquad** with respect to **v** ,**vu**, and **vu**, we can easily compute $\nabla\mathtt{w}$, the derivatives of **w** with respect to **x**. The "local" derivatives $(\frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{v}}, \frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{vu}}, \frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{vr}})$ can be computed efficiently by using the *reverse mode* of automatic differentiation. Here we maintain the derivative of the final result with respect to an intermediate quantity. These quantities are usually called *adjoints*. They measure the sensitivity of the final result with respect to some intermediate quantity. In the reverse mode, let **tbar** denote the adjoint object corresponding to **t**. The goal is for **tbar** to contain the derivative $\frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{t}}$. We know that $\mathtt{wbar} = \frac{\partial\,\mathtt{fquad}}{\partial\,\mathtt{fquad}} = 1.0$. We can compute **ybar** and **zbar** by applying the following simple rule to the statements executed in computing **fquad**, but in reverse order:

```
if s = f(t),   then tbar += sbar * (df/dt)
if s = f(t,u), then tbar += sbar * (df/dt)
                    ubar += sbar * (df/du)
```

Using this simple recipe (see [14,20]), we generate the code shown in Figure 3 for computing **vubar**, **vrbar**, and **vbar**. One can easily convince oneself that

$$\begin{aligned}\mathtt{vubar} &= 2 * \mathtt{hxy} * (\mathtt{vr} - \mathtt{v})\\ \mathtt{vrbar} &= 2 * \mathtt{hyx} * (\mathtt{vr} - \mathtt{v})\\ \mathtt{vbar} &= -2 * \mathtt{hxy} * (\mathtt{vu} - \mathtt{v}) - 2 * \mathtt{hyx} * (\mathtt{vr} - \mathtt{v})\end{aligned}$$

so that we have in fact computed the correct "local" derivatives. The code shown in Figure 2 has been generated by applying this same technique to all other assignments statements involving active variables and by optimizing the resulting code by removing additions with 0 and multiplications with 1. The ADIFOR-generated code for the whole subroutine is shown in Appendix B. ADIFOR is currently not consistent about pulling loop invariant subexpressions out of the loop, but will do so reliably in the future.

3 Extending the Scope of the Compile-Time Reverse Mode

In this section, we explore extensions of the compile-time reverse mode to

- a sequence of assignment statements,
- a nested loop, and
- the whole program.

A closer look at the current ADIFOR-generated code in the preceding sections reveals a substantial time and space overhead associated with the computations of auxiliary gradients such as **g$v**, **g$vu**, and **g$vr**. In this section, we explore different ways for improving the overall computation of the gradient by extending the scope of the reverse mode.

```
  /* Compute function values */
   d$0 = (vr-v)
   d$4 = (vu-v)
   t1 = d$0 * d$0
   t2 = t1 * hyx
   t3 = d$4 * d$4
   t5 = t3 * hxy
   w  = t2 + t5

/* Initialize adjoint quantities */
      wbar = 1.0; t3bar = 0.0; t2bar = 0.0;
      t1bar = 0.0; d$0bar = 0.0; d$4bar = 0.0;

/* Adjoints for w = t2 + t5 */
   t2bar = t2bar + wbar * 1
   t5bar = t5bar + wbar * 1
/* Adjoints for t5 = t3 * hxy */
   t3bar = t3bar + t5bar * hxy
/* Adjoints for t3 = d$4 * d$4 */
   d$4   = d$4 + t3bar * d$4
   d$4   = d$4 + t3bar * d$4
/* Adjoints for t2 = t1 * hyx */
   t1bar = t1bar + t2bar * hyx
/* Adjoints for  t1 = d0*d0 */
   d$0   = d$0 + t1bar * d$0
   d$0   = d$0 + t1bar * d$0
/* Adjoints for d$4 = vu - v */
   vubar = vubar + d$4bar * 1
   vbar  = vbar  + d$4bar * (-1)
/* Adjoints for d$0 = (vr-v) */
   vrbar = vrbar + d$0bar * 1
   vbar  = vbar  + d$0bar * (-1)
```

Figure 3: Unoptimized Reverse Mode Computation

3.1 Case 1: Reverse Mode for Basic Blocks inside the Loop

In the program for the torsion problem, there are three loops: two for the computation of the quadratic part of the function and one for the computation of the linear part. Consider, for example, LOOP1. Each loop iteration can be viewed as a mapping

$$[\mathtt{x(k)}, \mathtt{x(k+1)}, \mathtt{x(k+nx)}, \mathtt{fquad}_{\mathtt{old}}] \longmapsto \mathtt{fquad}_{\mathtt{new}}.$$

We use the notation $\mathtt{fquad}_{\mathtt{old}}$ and $\mathtt{fquad}_{\mathtt{new}}$ to distinguish between the original and updated value of the variable **fquad**. Hence, if we know

$$\frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k)}},\ \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k+1)}},\ \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k+nx)}},\ \text{and}\ \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{fquad}_{\mathtt{old}}}, \tag{2}$$

then we can update $\nabla\mathtt{fquad}$ as follows:

$$\begin{aligned}\nabla\mathtt{fquad} &= \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k)}}\nabla\mathtt{fquad} + \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k+1)}}\nabla\mathtt{x(k+1)} \\ &\quad + \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{x(k+nx)}}\nabla\mathtt{x(k+nx)} + \frac{\partial\,\mathtt{fquad}_{\mathtt{new}}}{\partial\,\mathtt{fquad}_{\mathtt{old}}}\nabla\mathtt{fquad}.\end{aligned}$$

The derivatives in the equation (2) can easily be computed by applying the reverse mode to the loop body. The resulting code is shown in Figure 4. Note that each variable is assigned only once in each loop iteration. If this had not been the case, we would have had to save the sequence of values of variables that are overwritten by allocating some extra temporary variables. This extension of the scope of the reverse mode saved us 3 derivative vectors **g$v**, **g$vr**, and **g$vu**, and decreased the number of derivative vector operations from 10 to 4.

In general, we can apply this technique in a straightforward fashion to any piece of code that has only one entry and exit point and does not contain subroutine or function calls or loops. We call such a piece of code a *basic block*. We may have to introduce some temporaries to make sure that each variable is assigned only once (i.e., represents a unique *value*) in a basic block, but this requires at most as many scalar temporaries as there are lines of code, an insignificant increase of storage. The savings achieved by this technique depend on the particular code at hand, but, in general, will be the more pronounced the more statements a basic block contains. The code that results from applying this technique to the whole subroutine is shown in Appendix C.

3.2 Case 2 : Reverse Mode for the Whole Loop

In order to expand the scope of the compile-time reverse mode, the special structure of the torsion problem is important. Defining

$$\mathtt{t_k} := -\mathtt{hyx} * (\mathtt{vr} - \mathtt{v}) * *2 + \mathtt{hxy} * (\mathtt{vu} - \mathtt{v}) * *2$$

to be the value computed in loop iteration **k** to upgrade **fquad**, we can express

$$\mathtt{fquad} = \sum_{\mathtt{k=1}}^{\mathtt{(nx+1)(ny+1)}} \mathtt{t_k}. \tag{3}$$

```
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
         G$FQUAD(G$I$) = 0.0d0
      END DO
      DO 99998 J = 0,NY
         DO 99999 I = 0,NX
            K = NX* (J-1) + I
c
c     compute new contribution to sum
c
            V = 0.0
            VR = 0.0
            VU = 0.0
            IF (I.GE.1 .AND. J.GE.1) THEN
               V = X(K)
            END IF
            IF (I.LT.NX .AND. J.GT.0) THEN
               VR = X(K+1)
            END IF
            IF (I.GT.0 .AND. J.LT.NY) THEN
               VU = X(K+NX)
            END IF
C             fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2

c
c  reverse mode computation for computing derivatives of
c x(k), x(k+1), x(k+nx). We know that the deriv. of fquad_new
c       with respect to fquad_old is 1.
c
            D$0 = VR - V
            D$4 = VU - V
            FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
            VBAR = -2*HXY*D$4 - 2*HYX*D$0
            VUBAR = 2*HXY*D$4
            VRBAR = 2*HYX*D$0
            XKBAR = 0.0
            XK1BAR = 0.0
            XKNXBAR = 0.0
            IF (I.GE.1 .AND. J.GE.1) XKBAR = VBAR
            IF (I.LT.NX .AND. J.GT.0) XK1BAR = VRBAR
            IF (I.GT.0 .AND. J.LT.NY) XKNXBAR = VUBAR

c
c  Chain Rule to update derivatives of fquad w.r.t. x
c

            DO PP = 1,G$P$
               G$FQUAD(PP) = G$FQUAD(PP) + XKBAR*G$X(PP,K) +
     +                       XK1BAR*G$X(PP,K+1) +
     +                       XKNXBAR*G$X(PP,K+NX)
            END DO

99999    CONTINUE
   20    CONTINUE
99998 CONTINUE
```

Figure 4: Reverse Mode for Basic Block in LOOP1

Since v, vu, and vr are defined in terms of x(k+1), x(k+nx), and x(k), t_k is a function of these values, that is,

$$t_k = t_k(x(k+1), x(k+nx), x(k)).$$

Since no entry of x is overwritten in any of the loop iterations, t_k and t_l do not depend on each other for $k \neq l$, and we can compute the sum (3) in any order. In compiler terms, there are no loop-carried dependencies and this loop is a parallel loop.

Remember that the reverse mode implicitly assumes that we are able to trace the values computed during some computation in the reverse order. Hence, a loop that is not parallel would require us to save some intermediate values. However, for a parallel loop, it is sufficient simply to generate the reverse mode code for the loop body. But this is exactly what we already did in the preceding section, where we computed

$$\frac{\partial t_k}{\partial x(k+1)}, \frac{\partial t_k}{\partial x(k)}, \frac{\partial t_k}{\partial x(k+nx)}.$$

Now, since t_l and t_k do not depend on each other for $l \neq k$, the associativity of addition allows us to compute

$$\frac{d\text{fquad}}{dx(j)} = \frac{\partial t_{j-1}}{\partial x(j)} + \frac{\partial t_{j-nx}}{\partial x(j)} + \frac{\partial t_j}{\partial x(j)}$$

in a piecemeal fashion, as each of the iterations j, $j-1$, and $j-nx$ contributes to $\frac{\partial \text{fquad}}{\partial x(j)}$. The resulting code is shown in Figure 5. The xbar vector contains $\frac{d\text{fquad}}{dx}$ and components k+1, k, and k+nx are updated in iteration k. After the loop, we apply the chain rule to compute

$$\nabla \text{fquad} = \frac{d\text{fquad}}{dx} \cdot \nabla x.$$

This matrix-vector multiplication is performed using the BLAS routine DGEMV [13].

To summarize, we exploited the fact that

- loop iterations do not depend on each other, and
- the result of each loop enters into the dependent variable (fquad) in an additive fashion.

This allowed us to generate reverse mode code for the whole loop by simply generating reverse mode code for the loop body, and the forward mode propagation of the global derivatives could be moved outside of the loop.

Compared with the code in the previous section, we now have a multiplication of an g$p $\times$ (nx+1) (ny+1) matrix by a vector outside the loop instead of (nx+1)(ny+1) multiplications of an g$p $\times 4$ matrix by a vector multiplication inside a loop that is executed (nx+1) (ny+1) times, requiring roughly one-fourth the number of operations. Applying this technique to the whole subroutine results in the code shown in Appendix D.

3.3 Case 3 : The Full Reverse Mode

So far we exploited only the particular structure of the code in LOOP1, LOOP2, and LOOP3. On the other hand, $f(x)$ is the sum of the contributions computed in LOOP1, LOOP2, LOOP3,

```
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
          G$FQUAD(G$I$) = 0.0d0
      END DO
      DO I = 1,XBARSIZE
          XBAR(I) = 0.0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              VR = 0.0
              VU = 0.0
              IF (I.GE.1 .AND. J.GE.1) V = X(K)
              IF (I.LT.NX .AND. J.GT.0) VR = X(K+1)
              IF (I.GT.0 .AND. J.LT.NY) VU = X(K+NX)
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
              D$0 = VR - V
              D$4 = VU - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
              VUBAR = 2*HXY*D$4
              VRBAR = 2*HYX*D$0
              IF (I.GE.1 .AND. J.GE.1) XBAR(K) = XBAR(K) + VBAR
              IF (I.LT.NX .AND. J.GT.0) XBAR(K+1) = XBAR(K+1) + VRBAR
              IF (I.GT.0 .AND. J.LT.NY) XBAR(K+NX) = XBAR(K+NX) + VUBAR
99999     CONTINUE
   20     CONTINUE
99998 CONTINUE
c
c xbar is the vector of partial derivatives of the contribution
c to fquad with respect to x.  Since fquad was zero before this
c loop, the derivative d$fquad = g$x * xbar.
c
      CALL DGEMV('n',G$P$,XBARSIZE,1.0d0,G$X,LDG$X,XBAR,1,1.0d0,G$FQUAD,
     +           1)
```

Figure 5: Reverse Mode for the Whole Loop

and, in addition to being parallel loops themselves, these loops do not depend on each other. So, instead of computing

```
xbar(1:n) = 0;
/* Update xbar in LOOP1 */
d$fquad = g$x * xbar

xbar(1:n) = 0;
/* Update xbar in LOOP2 */
d$fquad = d$fquad + g$x * xbar

xbar(1:n) = 0;
/* Update xbar in LOOP2 */
d$fquad = d$fquad + g$x * xbar
```

we could simply keep on updating xbar in LOOP1, LOOP2, and LOOP3 and perform compute $\mathtt{d}fquad = gx$ ***** **xbar** once at the end. This is possible since none of these loops updates the vector **x**, and hence **g$x** remains unchanged. But we can go even further: Since in the forward mode, **g$x** is initialized to the identity, we can eliminate the final multiplication **g$fquad** = **g$x** $*$ **xbar** and simply assign return **xbar**. In this fashion, we have generated adjoint code for the whole subroutine, and the code for computing the gradient does not contain any vector operations.

It is important to note that we were able to do the full implementation of the reverse mode because

- each of the three loops is a parallel loop,
- the three loops do not depend on each other,
- the contribution computed inside each loop enters in the final result in an additive fashion, and
- the results of each of the three loops are added to achieve the final result.

The resulting reverse mode code for the torsion problem is shown in Appendix E. While we did not decrease the storage requirement any further compared with the preceding section, we saved another three loops of size **g$p nx ny**, and the run time of this program no longer depends on **g$p**.

4 Exploring Partial Separability

As was mentioned in the introduction, the torsion problem is a partially separable function $f : \mathbf{R}^n \rightarrow \mathbf{R}$, in that it can be expressed as

$$f(x) = \sum_{i=1}^{nb} f_i(x).$$

This structure can also be used advantageously in computing the (usually dense) gradient ∇f of f (see [9]). Assume that the code for computation of f looks as follows:

```
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

```
subroutine g$fn(n,x,g$x,ldg$x,fval,g$fval,ldg$fval).
```

To compute ∇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, in current ADIFOR, the cost of computing ∇f is of the order of n times the function evaluation.

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

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

we have the identities

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

where e is the vector of all ones, and J_g is the Jacobian of g. However, if most of the component functions f_i depend only on a few parameters x_j, the Jacobian of g is sparse, and this fact can be exploited advantageously.

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

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

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

$$J = \begin{pmatrix} \bigcirc & & & \\ \bigcirc & & & \diamond \\ & \triangle & & \diamond \\ & \triangle & \square & \\ & \triangle & \square & \end{pmatrix}.$$

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 computing sparse Jacobians is to identify so-called structurally orthogonal columns j_i of J (see [10]), that is, columns whose inner product is always zero, independent of the numerical values of their nonzero entries. 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, namely $\{f_1, f_2\}$, and the set of functions that depend nontrivially on x_2, namely $\{f_3, f_4, f_5\}$, are disjoint. Because of the graph-coloring approaches that are used to reveal this structure, one usually associates a "color" with every set of structurally orthogonal columns.

To exploit this sparsity structure, we recall that ADIFOR (ignoring transposes) computes $J \cdot S$, where S is a matrix with **g$p** columns. For our example, setting $S = I_{4\times4}$ will give us J at roughly four times the cost of evaluating f, but if we exploit the structural orthogonality and set

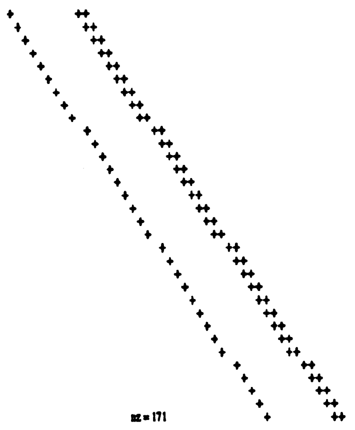
$$S = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix},$$

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

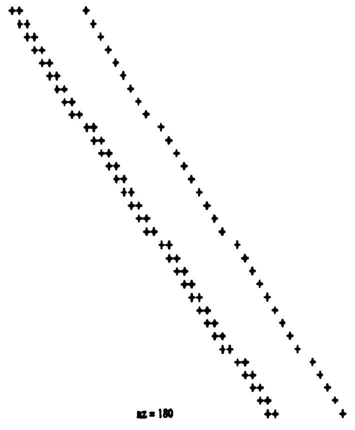
This idea can readily be applied to the torsion problem. By storing the contribution of iteration k to `fquad` in the `k`-th element of separate vectors `FQ`, `FQQ`, and `FP` (for the LOOP1, LOOP2, and LOOP3, respectively), the derivative of `fquad` is the sum of the row sums of the Jacobians of `FQ`, `FQQ`, and `FP`.

For example, the code for the loop corresponding to FQ is

```
      SUBROUTINE TORFCN1(N,X,X,F,NX,NY,HX,HY,FORCE,FQ)
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FQ(*),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION FQUAD,HXY,HYX,V,VR,VU
      INTEGER FQK,I,J,K
C     ..
      HXY = HX/HY
      HYX = HY/HX
      FQUAD = 0.0
      DO 20 J = 0,NY
          DO 10 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              VR = 0.0
```



g$FQ



g$FQQ

Figure 6: Sparsity Structures of Component Jacobians

```
               VU = 0.0
               IF (I.GE.1 .AND. J.GE.1) THEN
                   V = X(K)
               END IF
               IF (I.LT.NX .AND. J.GT.0) THEN
                   VR = X(K+1)
               END IF
               IF (I.GT.0 .AND. J.LT.NY) THEN
                   VU = X(K+NX)
               END IF
               FQK = (J* (NX+1)) + I + 1
               FQ(FQK) = HYX* (VR-V)**2 + HXY* (VU-V)**2
10         CONTINUE
20 CONTINUE
   END
```

The only change (compared with the corresponding code fragment in Appendix A) is that we replaced the accumulation of `fquad` by an assignment to `FQ`. Subroutines `torfcn2` and `torfcn3` to compute `FQQ` and `FP`, respectively, are generated in the same fashion. For these codes, ADIFOR then generates the derivative codes shown in Appendix F.

For $n = 40$, the structures of $\frac{d\mathtt{FQ}}{d\mathtt{x}}$ and $\frac{d\mathtt{FQQ}}{d\mathtt{x}}$ are shown in Figure 6, and $\frac{d\mathtt{FP}}{d\mathtt{x}}$ is diagonal. The Jacobian for FQ and FQQ can be grouped into three sets of structurally orthogonal columns, independent of the size of the problem. And in the case of the function FP, the Jacobian can be compressed into only one column.

Exploiting this structure, we can now initialize the gradient vector as follows:

```
*      ******************************************************************
*      * find sparsity pattern and compute compressed Jacobian pattern *
*      ******************************************************************

          CALL SPARSITY(N,X,F,NX,NY,HX,HY,INDROWQ,INDCOLQ,NNZQ,INDROWQQ,
     +                  INDCOLQQ,NNZQQ)

          DO I = 1,NNZQ
              INDROWQS(I) = INDROWQ(I)
              INDCOLQS(I) = INDCOLQ(I)
              INDROWQQS(I) = INDROWQQ(I)
              INDCOLQQS(I) = INDCOLQQ(I)
          END DO

          CALL DSM((NY+1)* (NX+1),N,NNZQ,INDROWQ,INDCOLQ,NGRPQ,MAXGRPQ,
     +             MINGRPQ,INFO,IPNTRQ,JPNTRQ,IWA,LIWA)

          CALL DSM((NX+1)* (NY+1),N,NNZQQ,INDROWQQ,INDCOLQQ,NGRPQQ,
     +             MAXGRPQQ,MINGRPQQ,INFO,IPNTRQQ,JPNTRQQ,IWA,LIWA)


*      *********************************************
*      * compute Jacobians for the individual loops *
*      *********************************************

c----- calc g$FQ
              DO I = 1,N
                  DO J = 1,MAXGRPQ
                      G$X(J,I) = 0
                  END DO
                  G$X(NGRPQ(I),I) = 1.0
              END DO
              CALL REVOA(MAXGRPQ,N,X,G$X,PMAX,F,NX,NY,HX,HY,FORCE,FQ,
     +                   G$FQ,MAXCOLOR)

c-------- calc g$FQQ
              DO I = 1,N
                  DO J = 1,MAXGRPQQ
                      G$X(J,I) = 0
                  END DO
                  G$X(NGRPQQ(I),I) = 1.0
              END DO
              CALL REVOB(MAXGRPQQ,N,X,G$X,PMAX,F,NX,NY,HX,HY,FORCE,FQQ,
     +                   G$FQQ,MAXCOLOR)

c------- calc G$FP
```

```
c ------ ngrpfp =1 as Jacobian is diagonal
              MAXGRPFP = 1
              DO I = 1,N
                 G$X(1,I) = 1.0
              END DO
              CALL REVOC(MAXGRPFP,N,X,G$X,PMAX,F,NX,NY,HX,HY,FORCE,FP,
     +                 G$FP,MAXCOLOR)

*      *********************************
*      * Assemble final gradient value *
*      *********************************


              DO I = 1,N
                 SPARSEGF(I) = 0.0e0
              END DO

              DO I = 1,NNZQ
                 ROW = INDROWQS(I)
                 COL = INDCOLQS(I)
                 SPARSEGF(COL) = SPARSEGF(COL) +
     +                           0.25*G$FQ(NGRPQ(COL),ROW)
              END DO

              DO I = 1,NNZQQ
                 ROW = INDROWQQS(I)
                 COL = INDCOLQQS(I)
                 SPARSEGF(COL) = SPARSEGF(COL) +
     +                           0.25*G$FQQ(NGRPQQ(COL),ROW)
              END DO

              TEMP = -FORCE*HX*HY
              DO K = 1,N
                 SPARSEGF(K) = SPARSEGF(K) + TEMP*G$FP(1,K)
              END DO
```

After we have initialized some arrays determining the sparsity pattern of the Jacobian, we call the MINPACK subroutine `DSM` [9] to determine the proper coloring for the Jacobians of `FQ` and `FQQ`. Having thus determined `NGRPQ(i)`, the "color" of column `i` and `MAXGRPQ`, the number of colors for the Jacobian of `FQ`, we initialize `g$x` and calls `rev0a` (a renamed version of the ADIFOR-generated subroutine for `torfcn1`) to compute the compressed Jacobian of FQ. The same idea is applied to compute `g$FQQ` and `g$FP`. Lastly, the derivative values of the subfunctions are all added into a sparse vector, without ever expanding the compressed component Jacobians, as shown below. For the Jacobian of `FQ`, the index arrays `INDROWQS` and `INDCOLQS` indicate the row and column index of nonzero entries, and the `NGRPQ` array indicates the group (corresponding to one particular color) of a certain column. The Jacobian of `FQQ` is dealt with accordingly. The uncompression of the Jacobian of FQ is trivial, since it was diagonal — we just add the i-th diagonal entry (properly scaled) to the i-th entry of the gradient accumulation vector SPARSEGF. The MINPACK documentation contains details on the particular data structures used to represent the sparse derivative matrices.

We note that we could of course apply the idea of the "basic block reverse mode" to generate improved derivative code for `torfcn1`, etc. This code is shown in Appendix G. We would expect much less spectacular savings in this case, since the length of the derivative objects was not more than three for our sparse Jacobians (whereas it was n when we did not exploit partial separability).

5 Experimental Results

We tested the performance of our various derivative codes on a Sun Sparcstation iPX with 48 Mbytes of memory and an IBM RS6000/550 with 128 Mbytes of memory. We computed gradients for $n = 10 * 10, 20 * 20, \ldots, 100 * 100$. For the alternatives described in Sections 2, 3.1, and 3.2, we computed gradients in slices of 10 elements (i.e., the gradient was computed by calling the derivative code $\lceil n/10 \rceil$ times). Figure 7 shows the ratio of the run time of a gradient to a function evaluation obtained for these derivative codes. As expected, the run time is linear in n, but the slope decreases as we expand the scope of the reverse mode.

In Figure 8 we show the ratio of the run time of a gradient to a function evaluation obtained by the full reverse mode (Section 3.3) and by exploiting the partial separability of the torsion problem. These graphs also show the run time of the handcoded derivative subroutine supplied in the MINPACK-2 test suite. We see that by exploiting partial separability, we can achieve very good performance for computing the gradient of the torsion problem. This is particularly noteworthy as we do not need to know anything more about the structure of the problem than that it is partially separable. In contrast, intimate knowledge of the code is required to develop the full reverse mode and the handcoded versions.

Acknowledgments

We thank Alan Carle, George Corliss, and Andreas Griewank for their comments. We are especially grateful to George Corliss for his thoughtful and thorough comments on an earlier draft of this paper.

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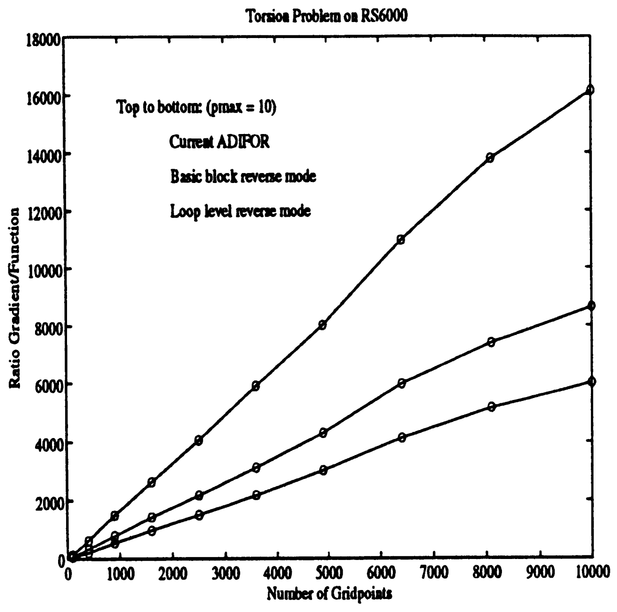


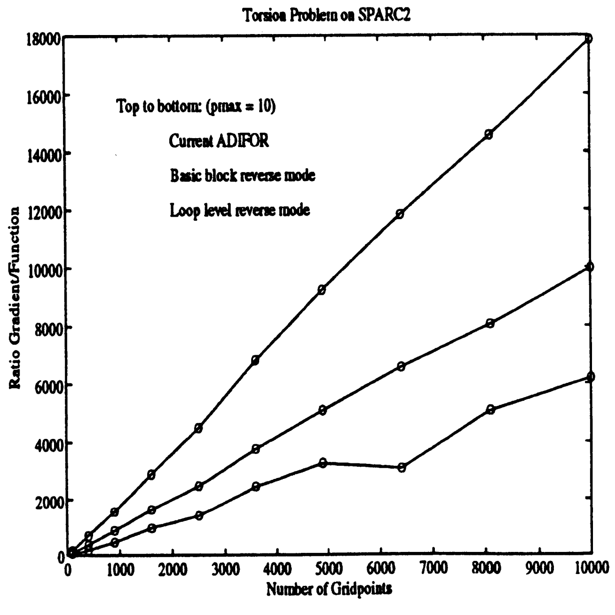
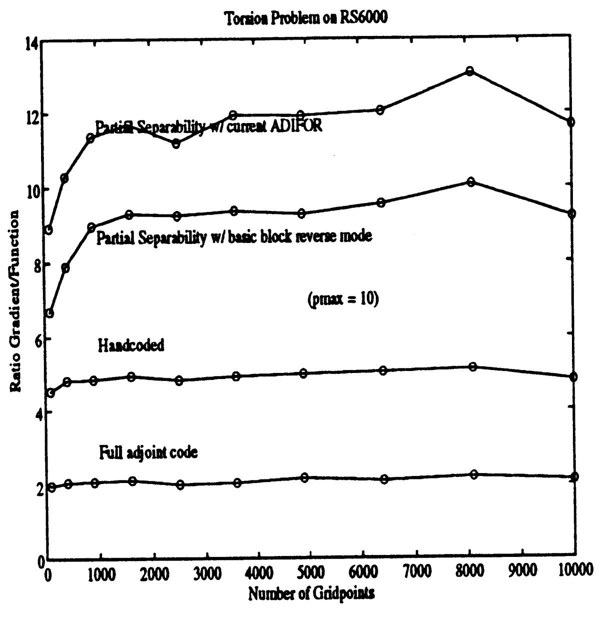


Figure 7: Performance of Current ADIFOR Code and Enhanced Versions



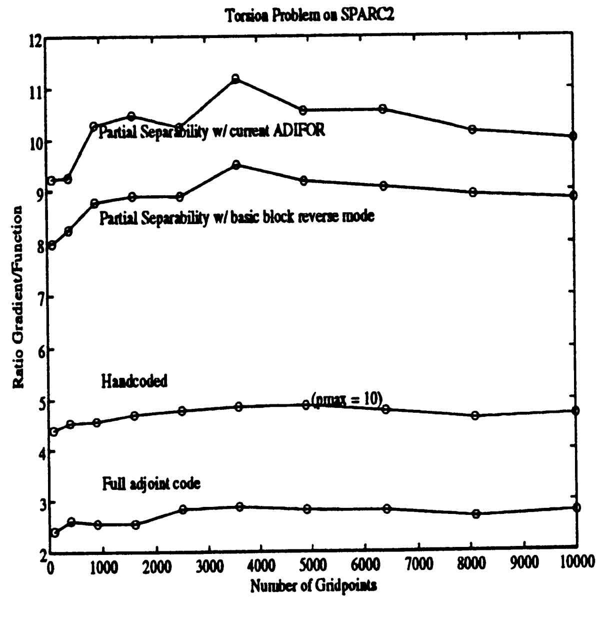


Figure 8: Exploiting Partial Separability, the Full Reverse Mode and Handcoded Derivatives

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APPENDICES: Code Listings for the Torsion Problem

A Minpack-2 Code for the Torsion Problem

```
      SUBROUTINE TORFCN(N,X,F,NX,NY,HX,HY,FORCE)

c     This subroutine computes the function of the torsion problem.

c     The spacing parameters hx and hy are for a rectangle with
c     nx points on the x-axis and ny points on the y-axis

C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION FLIN,FQUAD,HXY,HYX,V,VD,VL,VR,VU
      INTEGER I,J,K
C     ..
      HXY = HX/HY
      HYX = HY/HX

c     Computation of the quadratic part of the function.

c LOOP1:

      FQUAD = 0.0
      DO 20 J = 0,NY
          DO 10 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              VR = 0.0
              VU = 0.0
              IF (I.GE.1 .AND. J.GE.1) V = X(K)
              IF (I.LT.NX .AND. J.GT.0) VR = X(K+1)
              IF (I.GT.0 .AND. J.LT.NY) VU = X(K+NX)
              FQUAD = FQUAD + HYX* (VR-V)**2 + HXY* (VU-V)**2
   10     CONTINUE
   20 CONTINUE
c
c LOOP2:
c
      DO 40 J = 1,NY + 1
```

```
          DO 30 I = 1,NX + 1
              K = NX* (J-1) + I
              V = 0.0
              VL = 0.0
              VD = 0.0
              IF (I.LE.NX .AND. J.LE.NY) V = X(K)
              IF (I.GT.1 .AND. J.LE.NY) VL = X(K-1)
              IF (I.LE.NX .AND. J.GT.1) VD = X(K-NX)
              FQUAD = FQUAD + HYX* (VL-V)**2 + HXY* (VD-V)**2
   30     CONTINUE
   40 CONTINUE

c     Computation of the linear part of the function.

c LOOP 3:

      FLIN = 0.0
      DO 50 K = 1,NX*NY
          FLIN = FLIN + X(K)
   50 CONTINUE
      F = 0.25*FQUAD - FORCE*HX*HY*FLIN

      END
```

B Current ADIFOR Code for Torsion Problem

```
      SUBROUTINE REVO(G$P$,N,X,G$X,LDG$X,F,G$F,LDG$F,NX,NY,HX,HY,FORCE)
*****************************************************************
*
* generated by current ADIFOR for computing gradient of
* torsion problem. x independent, f dependent.
*
*****************************************************************
C
C       ADIFOR: runtime gradient index
C       ADIFOR: translation time gradient index
C       ADIFOR: gradient iteration index
C
C       **********
C       This subroutine computes the function of the torsion problem.
C       **********
C       The spacing parameters hx and hy are for a rectangle with
C       nx points on the x-axis and ny points on the y-axis
C
C       ADIFOR: gradient declarations
C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=4900)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$F,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION G$F(LDG$F),G$X(LDG$X,N),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FLIN,FQUAD,HXY,HYX,V,VD,VL,VR,VU
      INTEGER G$I$,I,J,K
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION G$FLIN(G$PMAX$),G$FQUAD(G$PMAX$),G$V(G$PMAX$),
     +                 G$VD(G$PMAX$),G$VL(G$PMAX$),G$VR(G$PMAX$),
     +                 G$VU(G$PMAX$)
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX
C       Computation of the quadratic part of the function.
```

```
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
          G$FQUAD(G$I$) = 0.0d0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              DO G$I$ = 1,G$P$
                  G$V(G$I$) = 0.0d0
              END DO
              VR = 0.0
              DO G$I$ = 1,G$P$
                  G$VR(G$I$) = 0.0d0
              END DO
              VU = 0.0
              DO G$I$ = 1,G$P$
                  G$VU(G$I$) = 0.0d0
              END DO
              IF (I.GE.1 .AND. J.GE.1) THEN
C                   v = x(k)
                  DO G$I$ = 1,G$P$
                      G$V(G$I$) = G$X(G$I$,K)
                  END DO
                  V = X(K)
              END IF
              IF (I.LT.NX .AND. J.GT.0) THEN
C                   vr = x(k + 1)
                  DO G$I$ = 1,G$P$
                      G$VR(G$I$) = G$X(G$I$,K+1)
                  END DO
                  VR = X(K+1)
              END IF
              IF (I.GT.0 .AND. J.LT.NY) THEN
C                   vu = x(k + nx)
                  DO G$I$ = 1,G$P$
                      G$VU(G$I$) = G$X(G$I$,K+NX)
                  END DO
                  VU = X(K+NX)
              END IF
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
              D$0 = VR - V
              D$4 = VU - V
              DO G$I$ = 1,G$P$
                  G$FQUAD(G$I$) = G$FQUAD(G$I$) + HYX*2*D$0*G$VR(G$I$) +
     +                            (- (HXY*2*D$4)- (HYX*2*D$0))*
     +                            G$V(G$I$) + HXY*2*D$4*G$VU(G$I$)
```

```
                 END DO
                 FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
   10            CONTINUE
99999       CONTINUE
   20       CONTINUE
99998 CONTINUE
        DO 99996 J = 1,NY + 1
            DO 99997 I = 1,NX + 1
                K = NX* (J-1) + I
                V = 0.0
                DO G$I$ = 1,G$P$
                    G$V(G$I$) = 0.0d0
                END DO
                VL = 0.0
                DO G$I$ = 1,G$P$
                    G$VL(G$I$) = 0.0d0
                END DO
                VD = 0.0
                DO G$I$ = 1,G$P$
                    G$VD(G$I$) = 0.0d0
                END DO
                IF (I.LE.NX .AND. J.LE.NY) THEN
C                     v = x(k)
                    DO G$I$ = 1,G$P$
                        G$V(G$I$) = G$X(G$I$,K)
                    END DO
                    V = X(K)
                END IF
                IF (I.GT.1 .AND. J.LE.NY) THEN
C                     vl = x(k - 1)
                    DO G$I$ = 1,G$P$
                        G$VL(G$I$) = G$X(G$I$,K-1)
                    END DO
                    VL = X(K-1)
                END IF
                IF (I.LE.NX .AND. J.GT.1) THEN
C                     vd = x(k - nx)
                    DO G$I$ = 1,G$P$
                        G$VD(G$I$) = G$X(G$I$,K-NX)
                    END DO
                    VD = X(K-NX)
                END IF
C                 fquad = fquad + hyx * (vl - v) ** 2 + hxy * (vd - v) ** 2
                D$0 = VL - V
                D$4 = VD - V
                DO G$I$ = 1,G$P$
                    G$FQUAD(G$I$) = G$FQUAD(G$I$) + HYX*2*D$0*G$VL(G$I$) +
     +                                  (- (HXY*2*D$4)- (HYX*2*D$0))*
     +                                  G$V(G$I$) + HXY*2*D$4*G$VD(G$I$)
               END DO
               FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
   30          CONTINUE
99997       CONTINUE
   40       CONTINUE
99996 CONTINUE
C       Computation of the linear part of the function.
      FLIN = 0.0
      DO G$I$ = 1,G$P$
          G$FLIN(G$I$) = 0.0d0
      END DO
      DO 99995 K = 1,NX*NY
C            flin = flin + x(k)
         DO G$I$ = 1,G$P$
             G$FLIN(G$I$) = G$FLIN(G$I$) + G$X(G$I$,K)
         END DO
         FLIN = FLIN + X(K)
   50    CONTINUE
99995 CONTINUE
C       f = 0.25 * fquad - force * hx * hy * flin
      DO G$I$ = 1,G$P$
          G$F(G$I$) = 0.25*G$FQUAD(G$I$) - (FORCE*HX*HY)*G$FLIN(G$I$)
      END DO
      F = 0.25*FQUAD - FORCE*HX*HY*FLIN
      END
```

C Reverse Mode for Basic Blocks

```
      SUBROUTINE REV1(G$P$,N,X,G$X,LDG$X,F,G$F,LDG$F,NX,NY,HX,HY,FORCE)
*******************************************
*
* reverse mode at basic block level
*
*******************************************
C
C        ADIFOR: runtime gradient index
C        ADIFOR: translation time gradient index
C        ADIFOR: gradient iteration index
C
C        **********
C        This subroutine computes the function of the torsion problem.
C        **********
C        The spacing parameters hx and hy are for a rectangle with
C        nx points on the x-axis and ny points on the y-axis
C
C        ADIFOR: gradient declarations
C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=10000)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$F,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION G$F(LDG$F),G$X(LDG$X,N),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FLIN,FLINBAR,FQUAD,HXY,HYX,V,VBAR,VD,
     +                 VDBAR,VL,VLBAR,VR,VRBAR,VU,VUBAR,XK1BAR,XKBAR,
     +                 XKNXBAR
      INTEGER G$I$,I,J,K,PP
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION G$FLIN(G$PMAX$),G$FQUAD(G$PMAX$)
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX
C        Computation of the quadratic part of the function.
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
          G$FQUAD(G$I$) = 0.0d0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
c
c     compute new contribution to sum
c
              V = 0.0
              VR = 0.0
              VU = 0.0
              IF (I.GE.1 .AND. J.GE.1) THEN
                  V = X(K)
              END IF
              IF (I.LT.NX .AND. J.GT.0) THEN
                  VR = X(K+1)
              END IF
              IF (I.GT.0 .AND. J.LT.NY) THEN
                  VU = X(K+NX)
              END IF
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2

c
c  reverse mode computation for computing derivatives of
c x(k), x(k+1), x(k+nx). We know that the deriv. of fquad_new
c       with respect to fquad_old is 1.
c
              D$0 = VR - V
              D$4 = VU - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
              VUBAR = 2*HXY*D$4
              VRBAR = 2*HYX*D$0
              XKBAR = 0.0
              XK1BAR = 0.0
              XKNXBAR = 0.0
              IF (I.GE.1 .AND. J.GE.1) XKBAR = VBAR
              IF (I.LT.NX .AND. J.GT.0) XK1BAR = VRBAR
              IF (I.GT.0 .AND. J.LT.NY) XKNXBAR = VUBAR

c
c  Chain Rule to update derivatives of fquad w.r.t. x
c

              DO PP = 1,G$P$
                  G$FQUAD(PP) = G$FQUAD(PP) + XKBAR*G$X(PP,K) +
     +                           XK1BAR*G$X(PP,K+1) +
     +                           XKNXBAR*G$X(PP,K+NX)
               END DO

99999       CONTINUE
   20       CONTINUE
99998 CONTINUE

      DO 99996 J = 1,NY + 1
          DO 99997 I = 1,NX + 1
              K = NX* (J-1) + I

              V = 0.0
              VL = 0.0
              VD = 0.0
              IF (I.LE.NX .AND. J.LE.NY) V = X(K)
              IF (I.GT.1 .AND. J.LE.NY) VL = X(K-1)
              IF (I.LE.NX .AND. J.GT.1) VD = X(K-NX)
C               fquad = fquad + hyx * (vl - v) ** 2 + hxy * (vd - v) ** 2

              D$0 = VL - V
              D$4 = VD - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
              VDBAR = 2*HXY*D$4
              VLBAR = 2*HYX*D$0
              XKBAR = 0.0
              XK1BAR = 0.0
              XKNXBAR = 0.0
              IF (I.LE.NX .AND. J.LE.NY) XKBAR = VBAR
              IF (I.GT.1 .AND. J.LE.NY) XK1BAR = VLBAR
              IF (I.LE.NX .AND. J.GT.1) XKNXBAR = VDBAR

              DO PP = 1,G$P$
                  G$FQUAD(PP) = G$FQUAD(PP) + XKBAR*G$X(PP,K) +
     +                          XK1BAR*G$X(PP,K-1) +
     +                          XKNXBAR*G$X(PP,K-NX)
              END DO
99997     CONTINUE
99996 CONTINUE


C       Computation of the linear part of the function.
      FLIN = 0.0
      DO G$I$ = 1,G$P$
          G$FLIN(G$I$) = 0.0d0
      END DO
      DO 99995 K = 1,NX*NY
cm          g$flin(k) = g$flin(k) + 1
          FLINBAR = 1.0
          DO I = 1,G$P$
              G$FLIN(I) = G$FLIN(I) + FLINBAR*G$X(I,K)
          END DO
          FLIN = FLIN + X(K)
99995 CONTINUE
C       f = 0.25 * fquad - force * hx * hy * flin
      DO G$I$ = 1,G$P$
          G$F(G$I$) = 0.25*G$FQUAD(G$I$) - (FORCE*HX*HY)*G$FLIN(G$I$)
      END DO
      F = 0.25*FQUAD - FORCE*HX*HY*FLIN
      END
```

D Reverse Mode for Loop Bodies

```
      SUBROUTINE REV2(G$P$,N,X,G$X,LDG$X,F,G$F,LDG$F,NX,NY,HX,HY,FORCE,
     +                XBAR,XBARSIZE)
************************
*
* reverse mode at individual loop level
*
************************
C
C        ADIFOR: runtime gradient index
C        ADIFOR: translation time gradient index
C        ADIFOR: gradient iteration index
C
C        **********
C        This subroutine computes the function of the torsion problem.
C        **********
C        The spacing parameters hx and hy are for a rectangle with
C        nx points on the x-axis and ny points on the y-axis
C
C        ADIFOR: gradient declarations

C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=10000)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$F,LDG$X,N,NX,NY,XBARSIZE
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION G$F(LDG$F),G$X(LDG$X,N),X(N),XBAR(*)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FLIN,FLINBAR,FQUAD,HXY,HYX,V,VBAR,VD,
     +                 VDBAR,VL,VLBAR,VR,VRBAR,VU,VUBAR
      INTEGER G$I$,I,J,K
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION G$FLIN(G$PMAX$),G$FQUAD(G$PMAX$)
C     ..
C     .. External Subroutines ..
      EXTERNAL DGEMV
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX
C       Computation of the quadratic part of the function.
      FQUAD = 0.0
      DO G$I$ = 1,G$P$
          G$FQUAD(G$I$) = 0.0d0
      END DO
      DO I = 1,XBARSIZE
          XBAR(I) = 0.0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              VR = 0.0
              VU = 0.0
              IF (I.GE.1 .AND. J.GE.1) V = X(K)
              IF (I.LT.NX .AND. J.GT.0) VR = X(K+1)
              IF (I.GT.0 .AND. J.LT.NY) VU = X(K+NX)
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
              D$0 = VR - V
              D$4 = VU - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
              VUBAR = 2*HXY*D$4
              VRBAR = 2*HYX*D$0
              IF (I.GE.1 .AND. J.GE.1) XBAR(K) = XBAR(K) + VBAR
              IF (I.LT.NX .AND. J.GT.0) XBAR(K+1) = XBAR(K+1) + VRBAR
              IF (I.GT.0 .AND. J.LT.NY) XBAR(K+NX) = XBAR(K+NX) + VUBAR
99999     CONTINUE
   20     CONTINUE
99998 CONTINUE
c
c xbar is the vector of partial derivatives of the contribution
c to fquad with respect to x.  Since fquad was zero before this
c loop, the derivative d$fquad = g$x * xbar.
c
       CALL DGEMV('n',G$P$,XBARSIZE,1.0d0,G$X,LDG$X,XBAR,1,1.0d0,G$FQUAD,
     +           1)

       DO I = 1,XBARSIZE
           XBAR(I) = 0.0
       END DO

       DO 99996 J = 1,NY + 1
           DO 99997 I = 1,NX + 1
               K = NX* (J-1) + I
```

```
                V = 0.0
                VL = 0.0
                VD = 0.0
                IF (I.LE.NX .AND. J.LE.NY) V = X(K)
                IF (I.GT.1 .AND. J.LE.NY) VL = X(K-1)
                IF (I.LE.NX .AND. J.GT.1) VD = X(K-NX)
C                 fquad = fquad + hyx * (vl - v) ** 2 + hxy * (vd - v) ** 2
                D$0 = VL - V
                D$4 = VD - V
                FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
                VBAR = -2*HXY*D$4 - 2*HYX*D$0
                VDBAR = 2*HXY*D$4
                VLBAR = 2*HYX*D$0
                IF (I.LE.NX .AND. J.LE.NY) XBAR(K) = XBAR(K) + VBAR
                IF (I.GT.1 .AND. J.LE.NY) XBAR(K-1) = XBAR(K-1) + VLBAR
                IF (I.LE.NX .AND. J.GT.1) XBAR(K-NX) = XBAR(K-NX) + VDBAR
99997      CONTINUE
99996 CONTINUE
c
c xbar is the vector of partial derivatives of the contribution
c to fquad with respect to x.  Since fquad was already initialized
c       before this loop, the derivative d$fquad = d$fquad + g$x * xbar.
c
      CALL DGEMV('n',G$P$,XBARSIZE,1.0d0,G$X,LDG$X,XBAR,1,1.0d0,G$FQUAD,
     +           1)

C       Computation of the linear part of the function.
      FLIN = 0.0
      DO G$I$ = 1,G$P$
          G$FLIN(G$I$) = 0.0d0
      END DO
      DO I = 1,XBARSIZE
          XBAR(I) = 0.0
      END DO

      DO 99995 K = 1,NX*NY
c          g$flin(k) = g$flin(k) + 1
          FLINBAR = 1.0
          XBAR(K) = XBAR(K) + FLINBAR
          FLIN = FLIN + X(K)
99995 CONTINUE
c
c     again, d$fquad = d$fquad + g$x * xbar.
c
      CALL DGEMV('n',G$P$,XBARSIZE,1.0d0,G$X,LDG$X,XBAR,1,1.0d0,G$FLIN,
     +           1)
C       f = 0.25 * fquad - force * hx * hy * flin
```

```
DO G$I$ = 1,G$P$
    G$F(G$I$) = 0.25*G$FQUAD(G$I$) - (FORCE*HX*HY)*G$FLIN(G$I$)
END DO
F = 0.25*FQUAD - FORCE*HX*HY*FLIN
END
```

E Reverse Mode for the Whole Program

```
      SUBROUTINE REV3(N,X,F,NX,NY,HX,HY,FORCE,XBAR,XBARSIZE)
C
C       ADIFOR: runtime gradient index
C       ADIFOR: translation time gradient index
C
C       **********
C       This subroutine computes the function of the torsion problem.
C       **********
C       The spacing parameters hx and hy are for a rectangle with
C       nx points on the x-axis and ny points on the y-axis
C
C       ADIFOR: gradient declarations

C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER N,NX,NY,XBARSIZE
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION X(N),XBAR(*)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FLIN,FLINBAR,FQUAD,HXY,HYX,T,V,VBAR,VD,
     +                 VDBAR,VL,VLBAR,VR,VRBAR,VU,VUBAR
      INTEGER I,J,K
C     ..
      HXY = HX/HY
      HYX = HY/HX
C       Computation of the quadratic part of the function.
      FQUAD = 0.0
      DO I = 1,XBARSIZE
          XBAR(I) = 0.0
      END DO
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              VR = 0.0
              VU = 0.0
              IF (I.GE.1 .AND. J.GE.1) V = X(K)
              IF (I.LT.NX .AND. J.GT.0) VR = X(K+1)
              IF (I.GT.0 .AND. J.LT.NY) VU = X(K+NX)
C               fquad = fquad + hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
              D$0 = VR - V
              D$4 = VU - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
```

```
            VUBAR = 2*HXY*D$4
            VRBAR = 2*HYX*D$0
            IF (I.GE.1 .AND. J.GE.1) XBAR(K) = XBAR(K) + VBAR
            IF (I.LT.NX .AND. J.GT.0) XBAR(K+1) = XBAR(K+1) + VRBAR
            IF (I.GT.0 .AND. J.LT.NY) XBAR(K+NX) = XBAR(K+NX) + VUBAR
99999     CONTINUE
99998 CONTINUE

      DO 99996 J = 1,NY + 1
          DO 99997 I = 1,NX + 1
              K = NX* (J-1) + I
              V = 0.0
              VL = 0.0
              VD = 0.0
              IF (I.LE.NX .AND. J.LE.NY) V = X(K)
              IF (I.GT.1 .AND. J.LE.NY) VL = X(K-1)
              IF (I.LE.NX .AND. J.GT.1) VD = X(K-NX)
C               fquad = fquad + hyx * (vl - v) ** 2 + hxy * (vd - v) ** 2
              D$0 = VL - V
              D$4 = VD - V
              FQUAD = FQUAD + HYX*D$0**2 + HXY*D$4**2
              VBAR = -2*HXY*D$4 - 2*HYX*D$0
              VDBAR = 2*HXY*D$4
              VLBAR = 2*HYX*D$0
              IF (I.LE.NX .AND. J.LE.NY) XBAR(K) = XBAR(K) + VBAR
              IF (I.GT.1 .AND. J.LE.NY) XBAR(K-1) = XBAR(K-1) + VLBAR
              IF (I.LE.NX .AND. J.GT.1) XBAR(K-NX) = XBAR(K-NX) + VDBAR
99997     CONTINUE
99996 CONTINUE
C       Computation of the linear part of the function.
      FLIN = 0.0
      T = - (FORCE*HX*HY)
cm    all the flinbar(k)'s are equal to 1.0
      FLINBAR = 1.0
      DO 99995 K = 1,NX*NY
          XBAR(K) = (0.25*XBAR(K)) + (T*FLINBAR)
          FLIN = FLIN + X(K)
99995 CONTINUE
      F = 0.25*FQUAD - FORCE*HX*HY*FLIN
      END
```

F Derivative Code for Component Functions

```
      SUBROUTINE REVOA(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FQ,G$FQ,
     +                 LDG$FQ)
**********
* derivative of first loop -- current ADIFOR
**********
C
C        Formal fq is active.
C        Formal x is active.
C
C
C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=100)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FQ,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FQ(*),G$FQ(LDG$FQ,*),G$X(LDG$X,N),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$0BAR,D$3,D$3BAR,FQUAD,HXY,HYX,V,VR,VU
      INTEGER FQK,G$I$,I,J,K
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION G$V(G$PMAX$),G$VR(G$PMAX$),G$VU(G$PMAX$)
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX
C       Computation of the quadratic part of the function.
      FQUAD = 0.0
      DO 99998 J = 0,NY
          DO 99999 I = 0,NX
              K = NX* (J-1) + I
              V = 0.0
              DO 99990 G$I$ = 1,G$P$
                  G$V(G$I$) = 0.0d0
99990         CONTINUE
              VR = 0.0
              DO 99989 G$I$ = 1,G$P$
                  G$VR(G$I$) = 0.0d0
```

```
99989        CONTINUE
             VU = 0.0
             DO 99988 G$I$ = 1,G$P$
                 G$VU(G$I$) = 0.0d0
99988        CONTINUE
             IF (I.GE.1 .AND. J.GE.1) THEN
C            v = x(k)
                 DO 99987 G$I$ = 1,G$P$
                     G$V(G$I$) = G$X(G$I$,K)
99987            CONTINUE
                 V = X(K)
             END IF
             IF (I.LT.NX .AND. J.GT.0) THEN
C            vr = x(k + 1)
                 DO 99986 G$I$ = 1,G$P$
                     G$VR(G$I$) = G$X(G$I$,K+1)
99986            CONTINUE
                 VR = X(K+1)
             END IF
             IF (I.GT.0 .AND. J.LT.NY) THEN
C            vu = x(k + nx)
                 DO 99985 G$I$ = 1,G$P$
                     G$VU(G$I$) = G$X(G$I$,K+NX)
99985            CONTINUE
                 VU = X(K+NX)
             END IF
C           m       fquad = fquad + hyx*(vr-v)**2 + hxy*(vu-v)**2
             FQK = (J* (NX+1)) + I + 1
C           fq(fqk) = hyx * (vr - v) ** 2 + hxy * (vu - v) ** 2
             D$0 = VR - V
             D$3 = VU - V
             D$3BAR = HXY* (2*D$3)
             D$0BAR = HYX* (2*D$0)
             DO 99984 G$I$ = 1,G$P$
                 G$FQ(G$I$,FQK) = D$0BAR*G$VR(G$I$) +
     +                            (-D$3BAR+ (-D$0BAR))*G$V(G$I$) +
     +                            D$3BAR*G$VU(G$I$)
99984        CONTINUE
             FQ(FQK) = HYX*D$0**2 + HXY*D$3**2
   10        CONTINUE
99999    CONTINUE
   20    CONTINUE
99998 CONTINUE
      END
      SUBROUTINE REVOB(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FQQ,G$FQQ,
     +                 LDG$FQQ)
**********
* derivs for second loop , current ADIFOR
**********
C
C        Formal fqq is active.
C        Formal x is active.
C
C
C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=100)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FQQ,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FQQ(*),G$FQQ(LDG$FQQ,*),G$X(LDG$X,N),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$0BAR,D$3,D$3BAR,HXY,HYX,V,VD,VL
      INTEGER FQK,G$I$,I,J,K
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION G$V(G$PMAX$),G$VD(G$PMAX$),G$VL(G$PMAX$)
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX
      DO 99998 J = 1,NY + 1
          DO 99999 I = 1,NX + 1
              K = NX* (J-1) + I
              V = 0.0
              DO 99990 G$I$ = 1,G$P$
                  G$V(G$I$) = 0.0d0
99990         CONTINUE
              VL = 0.0
              DO 99989 G$I$ = 1,G$P$
                  G$VL(G$I$) = 0.0d0
99989         CONTINUE
              VD = 0.0
              DO 99988 G$I$ = 1,G$P$
```

```
                    G$VD(G$I$) = 0.0d0
99988           CONTINUE
                IF (I.LE.NX .AND. J.LE.NY) THEN
C               v = x(k)
                    DO 99987 G$I$ = 1,G$P$
                        G$V(G$I$) = G$X(G$I$,K)
99987               CONTINUE
                    V = X(K)
                END IF
                IF (I.GT.1 .AND. J.LE.NY) THEN
C               vl = x(k - 1)
                    DO 99986 G$I$ = 1,G$P$
                        G$VL(G$I$) = G$X(G$I$,K-1)
99986               CONTINUE
                    VL = X(K-1)
                END IF
                IF (I.LE.NX .AND. J.GT.1) THEN
C               vd = x(k - nx)
                    DO 99985 G$I$ = 1,G$P$
                        G$VD(G$I$) = G$X(G$I$,K-NX)
99985               CONTINUE
                    VD = X(K-NX)
                END IF
C              m          fquad = fquad + hyx*(vl-v)**2 + hxy*(vd-v)**2
                FQK = ((J-1)* (NX+1)) + I
C              fqq(fqk) = hyx * (vl - v) ** 2 + hxy * (vd - v) ** 2
                D$0 = VL - V
                D$3 = VD - V
                D$3BAR = HXY* (2*D$3)
                D$0BAR = HYX* (2*D$0)
                DO 99984 G$I$ = 1,G$P$
                    G$FQQ(G$I$,FQK) = D$0BAR*G$VL(G$I$) +
     +                               (-D$3BAR+ (-D$0BAR))*G$V(G$I$) +
     +                               D$3BAR*G$VD(G$I$)
99984           CONTINUE
                FQQ(FQK) = HYX*D$0**2 + HXY*D$3**2
   30           CONTINUE
99999       CONTINUE
   40       CONTINUE
99998 CONTINUE
      END
      SUBROUTINE REV1C(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FP,RGFP,
     +                 LDG$FP)
***************
* third loop, basic block reverse mode
***************




C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FP,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FP(*),G$X(LDG$X,*),RGFP(LDG$FP,*),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION FPBAR,HXY,HYX
      INTEGER I,K
C     ..
      HXY = HX/HY
      HYX = HY/HX
c   Computation of the linear part of the function.

      DO 50 K = 1,NX*NY
          FPBAR = 1.0
          RGFP(1,K) = 0.0
          DO I = 1,G$P$
              RGFP(I,K) = RGFP(I,K) + FPBAR*G$X(I,K)
          END DO
          FP(K) = X(K)
   50 CONTINUE

      END
```

G Enhanced Derivative Code for Component Functions

```
      SUBROUTINE REV1A(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FQ,RGFQ,
     +                 LDG$FQ)
*********
* first loop contribution, basic block reverse mode
*********
C
C       ADIFOR: runtime gradient index
C       ADIFOR: translation time gradient index
C       ADIFOR: gradient iteration index
C
C       The spacing parameters hx and hy are for a rectangle with
C       nx points on the x-axis and ny points on the y-axis
C
C       ADIFOR: gradient declarations

C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=4900)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FQ,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FQ(*),G$X(LDG$X,N),RGFQ(LDG$FQ,*),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FQUAD,HXY,HYX,V,VBAR,VR,VRBAR,VU,VUBAR,
     +                 XK1BAR,XKBAR,XKNXBAR
      INTEGER FQK,I,J,K,PP
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF

      HXY = HX/HY
      HYX = HY/HX

c     Computation of the quadratic part of the function.a
c        the following  is not needed
c        do g$i$ = 1, g$p$
c          do j= 1, ((nx+1)*(ny+1))
c          rgfQ(g$i$,j) = 0.0d0
c        enddo
c        enddo
```

```
     FQUAD = 0.0
     DO 20 J = 0,NY
         DO 10 I = 0,NX
             K = NX* (J-1) + I
             V = 0.0
             VR = 0.0
             VU = 0.0
             IF (I.GE.1 .AND. J.GE.1) V = X(K)
             IF (I.LT.NX .AND. J.GT.0) VR = X(K+1)
             IF (I.GT.0 .AND. J.LT.NY) VU = X(K+NX)
             FQK = (J* (NX+1)) + I + 1
             FQ(FQK) = HYX* (VR-V)**2 + HXY* (VU-V)**2
             D$0 = VR - V
             D$4 = VU - V
             FQ(FQK) = HYX*D$0**2 + HXY*D$4**2
             VBAR = -2*HXY*D$4 - 2*HYX*D$0
             VUBAR = 2*HXY*D$4
             VRBAR = 2*HYX*D$0
             XKBAR = 0.0
             XK1BAR = 0.0
             XKNXBAR = 0.0
             IF (I.GE.1 .AND. J.GE.1) XKBAR = VBAR
             IF (I.LT.NX .AND. J.GT.0) XK1BAR = VRBAR
             IF (I.GT.0 .AND. J.LT.NY) XKNXBAR = VUBAR

             DO PP = 1,G$P$
                 RGFQ(PP,FQK) = XKBAR*G$X(PP,K) + XK1BAR*G$X(PP,K+1) +
     +                          XKNXBAR*G$X(PP,K+NX)
             END DO
10       CONTINUE
20   CONTINUE
     END
```

```
      SUBROUTINE REV1B(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FQQ,RGFQQ,
     +                 LDG$FQQ)
***********
*  second loop, basic block reverse mode
***********
C
C       ADIFOR: runtime gradient index
C       ADIFOR: translation time gradient index
C       ADIFOR: gradient iteration index
C
C       The spacing parameters hx and hy are for a rectangle with
C       nx points on the x-axis and ny points on the y-axis
C
C       ADIFOR: gradient declarations

C     .. Parameters ..
      INTEGER G$PMAX$
      PARAMETER (G$PMAX$=4900)
C     ..
C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FQQ,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FQQ(*),G$X(LDG$X,N),RGFQQ(LDG$FQQ,*),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION D$0,D$4,FQUAD,HXY,HYX,V,VBAR,VD,VDBAR,VL,VLBAR,
     +                 XK1BAR,XKBAR,XKNXBAR
      INTEGER FQK,I,J,K,PP
C     ..
      IF (G$P$.GT.G$PMAX$) THEN
          PRINT *,'Parameter g$p is greater than g$pmax.'
          STOP
      END IF
      HXY = HX/HY
      HYX = HY/HX

c     Computation of the quadratic part of the function.
c        the following is NOT needed
c        do g$i$ = 1, g$p$
c         do j= 1, ((nx+1)*(ny+1))
c          rgfQQ(g$i$,j) = 0.0d0
c        enddo
c        enddo
      FQUAD = 0.0
      DO 40 J = 1,NY + 1
```

```
          DO 30 I = 1,NX + 1
             K = NX* (J-1) + I
             V = 0.0
             VL = 0.0
             VD = 0.0
             IF (I.LE.NX .AND. J.LE.NY) V = X(K)
             IF (I.GT.1 .AND. J.LE.NY) VL = X(K-1)
             IF (I.LE.NX .AND. J.GT.1) VD = X(K-NX)
cm          fquad = fquad + hyx*(vl-v)**2 + hxy*(vd-v)**2
             FQK = ((J-1)* (NX+1)) + I
             FQQ(FQK) = HYX* (VL-V)**2 + HXY* (VD-V)**2
             D$0 = VL - V
             D$4 = VD - V
             FQQ(FQK) = HYX*D$0**2 + HXY*D$4**2
             VBAR = -2*HXY*D$4 - 2*HYX*D$0
             VLBAR = 2*HYX*D$0
             VDBAR = 2*HXY*D$4
             XKBAR = 0.0
             XK1BAR = 0.0
             XKNXBAR = 0.0
             IF (I.LE.NX .AND. J.LE.NY) XKBAR = VBAR
             IF (I.GT.1 .AND. J.LE.NY) XK1BAR = VLBAR
             IF (I.LE.NX .AND. J.GT.1) XKNXBAR = VDBAR

             DO PP = 1,G$P$
                RGFQQ(PP,FQK) = XKBAR*G$X(PP,K) + XK1BAR*G$X(PP,K-1) +
     +                          XKNXBAR*G$X(PP,K-NX)
             END DO

 30       CONTINUE
 40    CONTINUE
       END
```

```
      SUBROUTINE REV1C(G$P$,N,X,G$X,LDG$X,F,NX,NY,HX,HY,FORCE,FP,RGFP,
     +                 LDG$FP)
****************
* third loop, basic block reverse mode
****************



C     .. Scalar Arguments ..
      DOUBLE PRECISION F,FORCE,HX,HY
      INTEGER G$P$,LDG$FP,LDG$X,N,NX,NY
C     ..
C     .. Array Arguments ..
      DOUBLE PRECISION FP(*),G$X(LDG$X,*),RGFP(LDG$FP,*),X(N)
C     ..
C     .. Local Scalars ..
      DOUBLE PRECISION FPBAR,HXY,HYX
      INTEGER I,K
C     ..
      HXY = HX/HY
      HYX = HY/HX
c   Computation of the linear part of the function.

      DO 50 K = 1,NX*NY
          FPBAR = 1.0
          RGFP(1,K) = 0.0
          DO I = 1,G$P$
              RGFP(I,K) = RGFP(I,K) + FPBAR*G$X(I,K)
          END DO
          FP(K) = X(K)
   50 CONTINUE

      END
```