Derivatives

Minimisation of a cost function $\rightarrow \nabla_x J_0$

$$J_o(x) = \sum_{i=1}^{N} \| H(\underbrace{M(M(\ldots M(x)))}_{k(i)\,times}) - y_i \|_R^{\,2}$$

- R is the observation error correlation matrix ($\|X\|_R^2 = XR^{-1}X$),
- M is the `croco step`,
- x the control vector,
- H an observation operator,
- $y_1, y_2, \ldots y_N$ observations.

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Automatic differentiation, cf RT Tapenade

A program P of a function F is a sequence of instructions:

$$P: \{I_1; I_2; \ldots; I_p\}$$

Each I_k implements an elementary vector function f_k

$$F = f_p \circ f_{p-1} \cdots \circ f_1$$

So the derivation of F may be computed with the chain rule

$$F'(X) = f'_p(f_{p-1}(f_{p-2}(\ldots))) \times f'_{p-1}(f_{p-2}(\ldots)) \ldots f'_2(f_1(X)) \times f'_1(X)$$

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$$F'(X) = \begin{pmatrix} \frac{\partial F_1}{\partial x_1}|X & \frac{\partial F_1}{\partial x_2}|X & \cdots & \frac{\partial F_1}{\partial x_n}|X \\ \frac{\partial F_2}{\partial x_1}|X & \frac{\partial F_2}{\partial x_2}|X & \cdots & \frac{\partial F_2}{\partial x_n}|X \\ & & \cdots & \\ \frac{\partial F_n}{\partial x_1}|X & \frac{\partial F_n}{\partial x_2}|X & \cdots & \frac{\partial F_n}{\partial x_n}|X \end{pmatrix}$$

With $X_0 = X$ and for $k > 1$, $X_k = f_k(X_{k-1})$

- tangent linear model, forward mode, column access

$$TLM(F, X) : v \to F'(X) \times v = f'_p(X_{p-1}) \times f'_{p-1}(X_{p-2}) \cdots \times f'_1(X_0) \times v$$

- adjoint model, reverse mode, line access

$$ADJ(F', X) : u \to F'(X)^t \times u = f'_1(X_0)^t \times f'_2(X_1)^t \cdots \times f'_p(X_{p-1})^t \times u$$

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real x,y
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Elementary functions

$$X = \begin{pmatrix} x \\ y \end{pmatrix}$$

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TLM & ADJ

$$X_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, X_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$TLM : f_2(f_1(X)) \times f_1'(X) \times X_0$$

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CALL PUSHREAL4(x)
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croco AD status (https://gitlab.inria.fr/bremond/croco)

Differentiation of croco 2D and some part of croco 3D

- ad-seq-friction-tide : sequential control of Cb in a configuration similar to DAS & LARDNER
- ad-par-friction-tide : parallel (MPI) control of Cb
- to-tapenade3.14 : North Atlantic config, control of a spatialized z0b (dyneco_rec) (cf Martial Boutet thesis)
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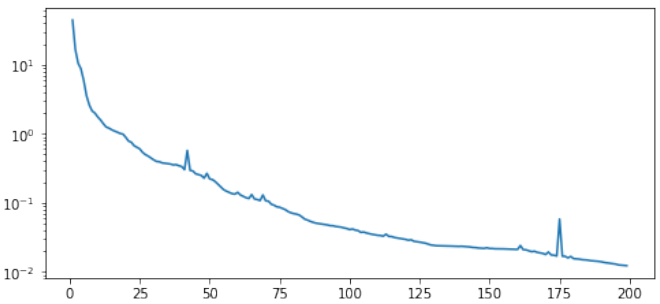
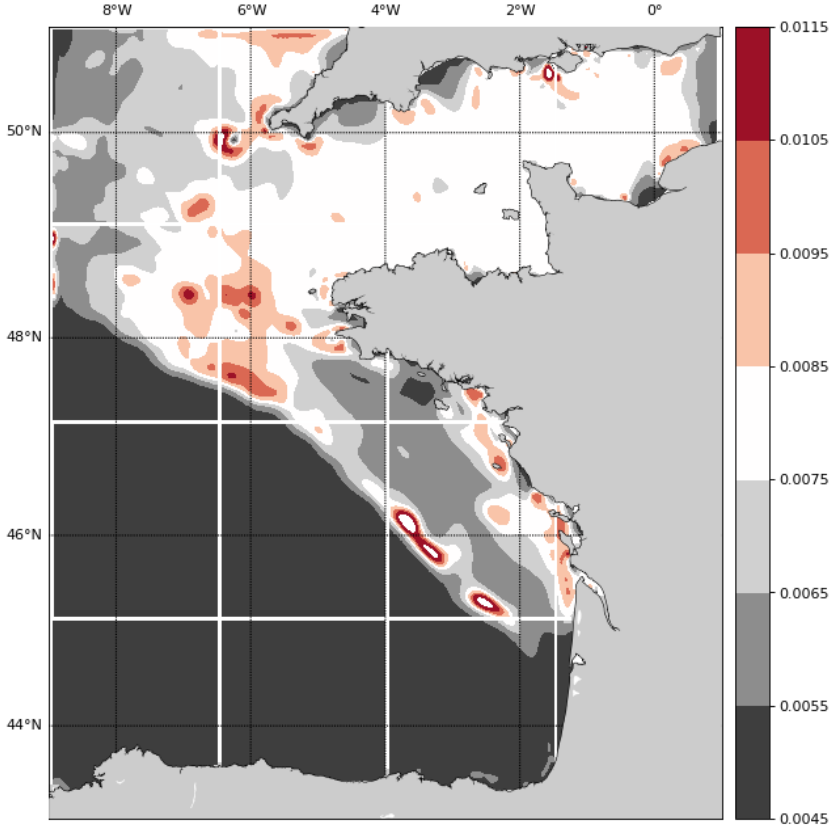
Differentiation of croco 2D



Cost (m^2)



z0b (mm)

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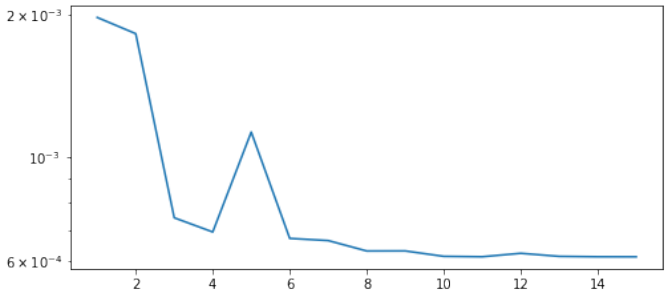
Differentiation of croco 3D



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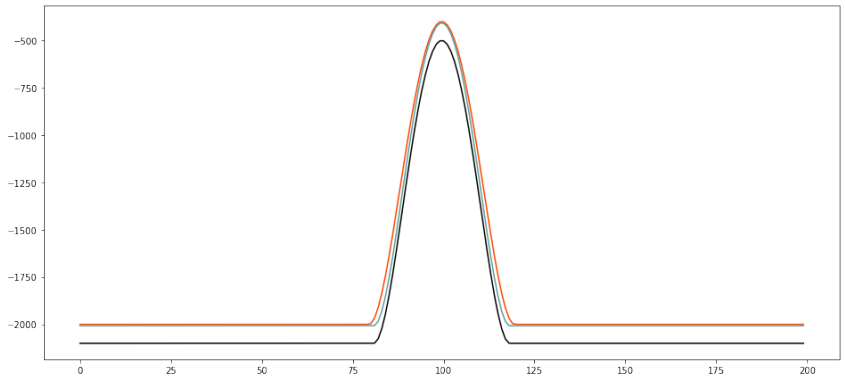
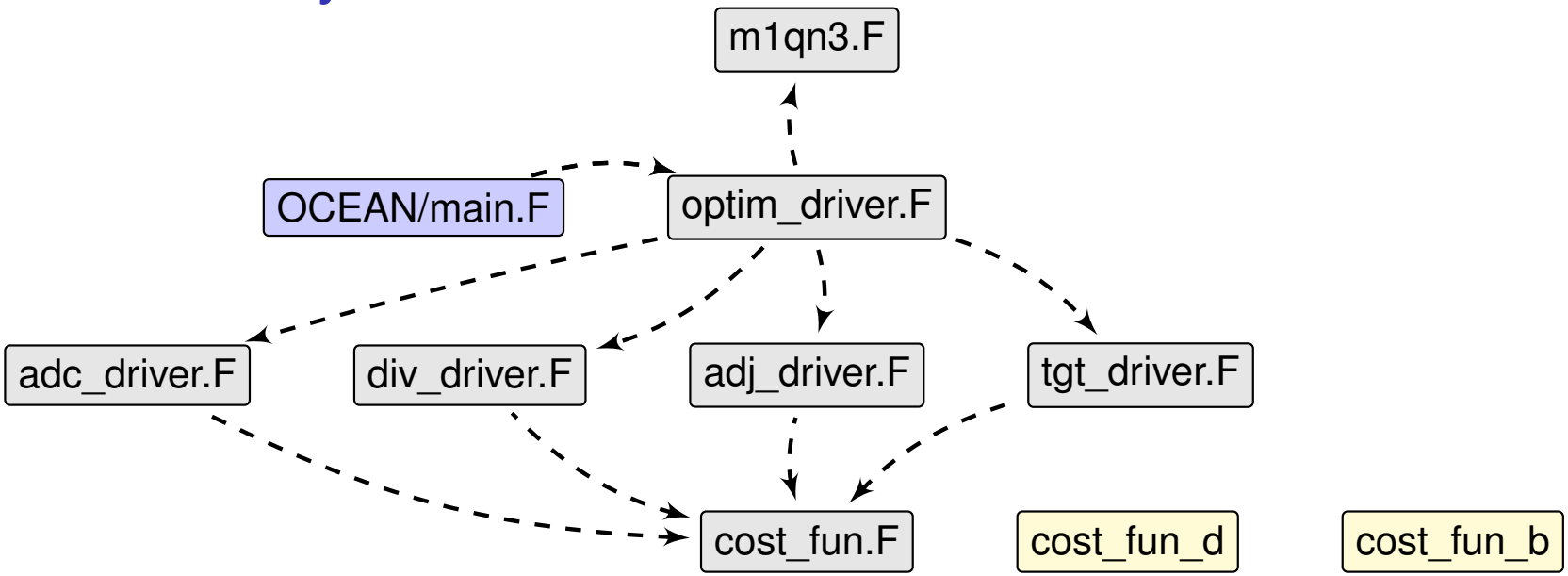


penalization layer

AD code organization

AD directory



Compile directory

Tapenade

Compile/autodiff_d.F

Compile/autodiff_b.F

Makefile targets

croco

croco_adc

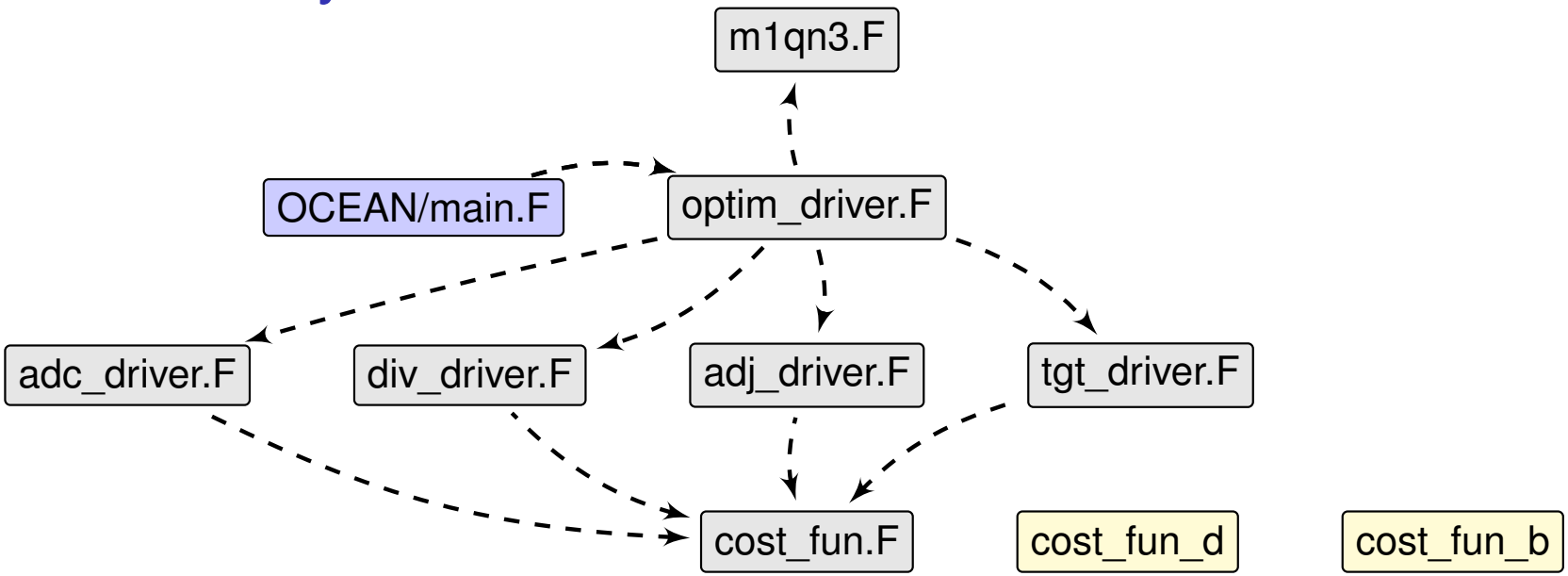
croco_div

croco_tgt

croco_adj

AD code organization

AD directory



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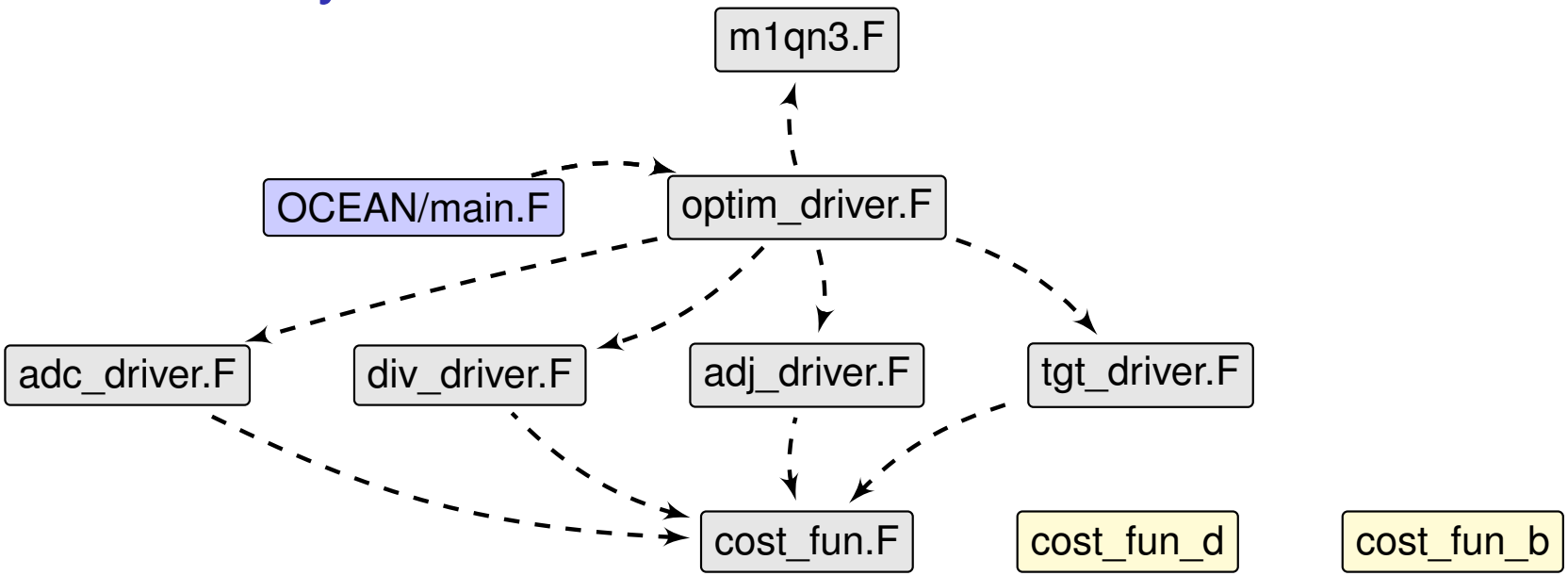

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Configuration specific

adparam.h read_obs.F write_obs.F save_restore.F set_state.F

- `adparam.h`: parameters (size of the problem, of assimilation window, etc.),
- `save_restore`: full croco state,
- `set_state`: from control vector (`ad_x`) to croco state.

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AD code organization

Tangent driver

```
do i=1,Sn
    ad_xd(i) = 1
    cost = icost
    idfdx = grad(i)
    call save_croco_state()
    write (*,*) '--------------------------------------'
    write (*,*) 'start tangent:',i
    write (*,*) '--------------------------------------'
    call cost_fun_d(ad_x, ad_xd, cost, idfdx)

    write (*,*) '--------------------------------------'
    write (*,*) 'end tangent:',i
    write (*,*) '--------------------------------------'
    call restore_croco_state()
    ad_xd(i) = 0
    grad(i)  = idfdx
 end do
```

AD code organization

Adjoint driver

```
call save_croco_state()
write (*,*) '--------------------------------------'
write (*,*) 'start cost'
write (*,*) '--------------------------------------'
call cost_fun(ad_x, icost)
cost = icost
write (*,*) '--------------------------------------'
write (*,*) 'end cost:'
write (*,*) '--------------------------------------'
call restore_croco_state()

call save_croco_state()
write (*,*) '--------------------------------------'
write (*,*) 'start adjoint'
write (*,*) '--------------------------------------'
ad_g(:) = 0.
costb = 1
call cost_fun_b(ad_x, ad_g, icost, costb)
write (*,*) '--------------------------------------'
write (*,*) 'end adjoint:'
write (*,*) '--------------------------------------'
call restore_croco_state()
```

Some issues for code writing:

1. non differentiable functions,
2. checkpointing of unused parts of arrays,
3. more checkpoints with temporary variables,
4. independent iterations loop,
5. global control of checkpointing.

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Non differentiable functions

Non differentiable functions

Euclidian distance function

```
function f(x,y)

implicit none
real f,x,y

f = sqrt(x*x + y*y)

end function f
```

Tapenade adjoint

```
REAL tempb
IF (x**2 + y**2 .EQ. 0.0) THEN
  tempb = 0.0
ELSE
  tempb = fb/(2.0*SQRT(x**2+y**2))
END IF
xb = xb + 2*x*tempb
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function f(x)
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```
      FUNCTION F_D(x, xd, f)
      IMPLICIT NONE

C
      REAL x, f
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C
      IF (x .EQ. 1) THEN
        f = 1
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derivative is 0 at 1

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Checkpointing of unused parts of arrays

Only a part of x is used

```
subroutine f(x)

implicit none
real x(999,999)
integer i

do i=2,4,1
  call step(x,i)
end do

end subroutine f

subroutine step(x,i)
implicit none
real x(999,999)

integer i

x(i,1) = x(i-1,1) + x(i-1,1)*x(i-1,1)

end subroutine step
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Tapenade adjoint

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SUBROUTINE F_B(x, xb)
IMPLICIT NONE
REAL x(999, 999)
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INTEGER i

DO i=2,4,1
  CALL PUSHREAL4ARRAY(x, 999**2)
  CALL STEP(x, i)
ENDDO
DO i=4,2,-1
  CALL POPREAL4ARRAY(x, 999**2)
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Solution here

use a C$AD NOCHECKPOINT on step

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use a `C$AD NOCHECKPOINT` on step

More checkpoints with temp variables

Direct update

```
subroutine f(x)
implicit none
real x,cff1,cff2
integer i

do i=1,2
   x=x+x*x
end do
```

Adjoint

```
DO i=1,2
  CALL PUSHREAL4(x)
  x = x + x*x
ENDDO
DO i=2,1,-1
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  xb = (2*x+1.0)*xb
ENDDO
```

With a temp variable

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implicit none
real x,cff1,cff2
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   x=x+cff2
end do
end subroutine f
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DO i=1,2
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ENDDO
DO i=2,1,-1
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  cff2b = xb
  cff1b = x*cff2b
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DO i=1,2
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  cff1 = x
  cff2 = cff1*x
  CALL PUSHREAL4(x)
  x = x + cff2
ENDDO
DO i=2,1,-1
  CALL POPREAL4(x)
  cff2b = xb
  cff1b = x*cff2b
  xb = xb + cff1b + cff1*cff2b
  CALL POPREAL4(cff1)
ENDDO
```

More checkpoints with temp variables

Direct update

```
subroutine f(x)
implicit none
real x,cff1,cff2
integer i

do i=1,2
   x=x+x*x
end do
```

With a temp variable

```
subroutine f(x)
implicit none
real x,cff1,cff2
integer i
do i=1,2
   cff1=x
   cff2=cff1*x
   x=x+cff2
end do
end subroutine f
```

Adjoint

```
DO i=1,2
  CALL PUSHREAL4(x)
  x = x + x*x
ENDDO
DO i=2,1,-1
  CALL POPREAL4(x)
  xb = (2*x+1.0)*xb
ENDDO
```

Adjoint

```
DO i=1,2
  CALL PUSHREAL4(cff1)
  cff1 = x
  cff2 = cff1*x
  CALL PUSHREAL4(x)
  x = x + cff2
ENDDO
DO i=2,1,-1
  CALL POPREAL4(x)
  cff2b = xb
  cff1b = x*cff2b
  xb = xb + cff1b + cff1*cff2b
  CALL POPREAL4(cff1)
ENDDO
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Solution here: !$acc loop directive

```
!$acc loop
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
```

Again...

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Solution here: !$TLOOP directive

Again

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Solution here: !$acc loop directive

Again

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Solution here: II-LOOP directive

```
C$AD   II-LOOP
       do i = 2,4,2
          x(i) = x(i-1)*x(i-1)
       end do
```

Adjoint

```
      SUBROUTINE F_B(x, xb)
      IMPLICIT NONE
      REAL x(4)
      REAL xb(4)
      INTEGER i
C$BWD-OF II-LOOP
      DO i=2,4,2
        xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
        xb(i) = 0.0
      ENDDO
      END
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Solution here: II-LOOP directive

```
C$AD  II-LOOP
      do i = 2,4,2
         x(i) = x(i-1)*x(i-1)
      end do
```

Adjoint

```
      SUBROUTINE F_B(x, xb)
      IMPLICIT NONE
      REAL x(4)
      REAL xb(4)
      INTEGER i
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      DO i=2,4,2
        xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
        xb(i) = 0.0
      ENDDO
      END
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Solution here: II-LOOP directive

```
C$AD  II-LOOP
      do i = 2,4,2
         x(i) = x(i-1)*x(i-1)
      end do
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Adjoint

```
SUBROUTINE F_B(x, xb)
IMPLICIT NONE
REAL x(4)
REAL xb(4)
INTEGER i
C$BWD-OF II-LOOP
DO i=2,4,2
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
implicit none
real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Solution here: II-LOOP directive

```
C$AD  II-LOOP
      do i = 2,4,2
         x(i) = x(i-1)*x(i-1)
      end do
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
  CALL POPREAL4(x(i))
  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Adjoint

```
      SUBROUTINE F_B(x, xb)
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      REAL x(4)
      REAL xb(4)
      INTEGER i
C$BWD-OF II-LOOP
      DO i=2,4,2
        xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
        xb(i) = 0.0
      ENDDO
      END
```

Independent iterations : simple example

Update at even indices

```
subroutine f(x)
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real x(4)
integer i
do i = 2,4,2
   x(i) = x(i-1)*x(i-1)
end do
end subroutine f
```

Solution here: II-LOOP directive

```
C$AD  II-LOOP
      do i = 2,4,2
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      end do
```

Tapenade adjoint

```
DO i=2,4,2
  CALL PUSHREAL4(x(i))
  x(i) = x(i-1)*x(i-1)
ENDDO
DO i=4,2,-2
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  xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
  xb(i) = 0.0
ENDDO
END
```

Adjoint

```
      SUBROUTINE F_B(x, xb)
      IMPLICIT NONE
      REAL x(4)
      REAL xb(4)
      INTEGER i
C$BWD-OF II-LOOP
      DO i=2,4,2
        xb(i-1) = xb(i-1) + 2*x(i-1)*xb(i)
        xb(i) = 0.0
      ENDDO
      END
```

Dependent iterations : example in cost_fun.F

croco step call

```
C$AD BINOMIAL-CKP ad_nt+1 40 1
      do ta=1,ad_nt
         do xk=1,ad_ns
            call step()
         end do
         call cost_fun_step(ad_x_f,cost,ta)
      end do
```

- control of the maximum number q of allowed snapshots (here $q = 40$)
- The time required to compute the adjoint grows like the q-th root of ad_nt.
- config ATLN with 40 allowed snapshots, $ad\_nt = 80$, $ad\_ns = 180$: time of adjoint computation is 3.5 the time of model.

Dependent iterations : example in cost_fun.F

croco step call

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C$AD BINOMIAL-CKP ad_nt+1 40 1
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Dependent iterations : example in cost_fun.F

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Dependent iterations : example in cost_fun.F

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- The time required to compute the adjoint grows like the q-th root of ad_nt.
- config ATLN with 40 allowed snapshots, $ad\_nt = 80$, $ad\_ns = 180$: time of adjoint computation is 3.5 the time of model.

Aliasing

Example pre_step3D

```
            call pre_step3d_tile (Istr,Iend,Jstr,Jend,
     &                A3d(1,1,trd), A3d(1,2,trd), A3d(1,3,trd),
     &                A2d(1,1,trd), A2d(1,2,trd), A2d(1,3,trd),
# ifdef VADV_ADAPT_IMP
     &                                            A2d(1,4,trd),
# endif
     &                A2d(1,1,trd), A2d(1,2,trd), A2d(1,3,trd)
#ifdef OPENACC
     &   ,A3d(1,4,trd),A3d(1,5,trd),A3d(1,6,trd),A3d(1,7,trd)
#endif
     &                                          , A3d(1,8,trd)
     &                                                       )
```

Unaliasing

```
            call pre_step3d_tile (Istr,Iend,Jstr,Jend,
     &                ad_x_ru(:,trd),ad_x_rv(:,trd),ad_x_rw(:,trd),
     &                ad_x_FC(:,trd),ad_x_CF(:,trd),ad_x_DC(:,trd),
# ifdef VADV_ADAPT_IMP
     &                                            ad_x_WC(:,4,trd),
# endif
     &                ad_x_FX(:,trd), ad_x_FE(:,trd), ad_x_WORK(:,trd)
     &                                          , ad_x_Hz_half(:,trd)
     &                                                       )
```

Aliasing

Example pre_step3D

```
            call pre_step3d_tile (Istr,Iend,Jstr,Jend,
     &                A3d(1,1,trd), A3d(1,2,trd), A3d(1,3,trd),
     &                A2d(1,1,trd), A2d(1,2,trd), A2d(1,3,trd),
# ifdef VADV_ADAPT_IMP
     &                                            A2d(1,4,trd),
# endif
     &                A2d(1,1,trd), A2d(1,2,trd), A2d(1,3,trd)
#ifdef OPENACC
     &   ,A3d(1,4,trd),A3d(1,5,trd),A3d(1,6,trd),A3d(1,7,trd)
#endif
     &                                          , A3d(1,8,trd)
     &                                                       )
```

Unaliasing

```
           call pre_step3d_tile (Istr,Iend,Jstr,Jend,
     &                ad_x_ru(:,trd),ad_x_rv(:,trd),ad_x_rw(:,trd),
     &                ad_x_FC(:,trd),ad_x_CF(:,trd),ad_x_DC(:,trd),
# ifdef VADV_ADAPT_IMP
     &                                            ad_x_WC(:,4,trd),
# endif
     &                ad_x_FX(:,trd), ad_x_FE(:,trd), ad_x_WORK(:,trd)
     &                                          , ad_x_Hz_half(:,trd)
     &                                                       )
```