Cryana Tutorial

In this tutorial you can find the way to get Cryana from ParamagneticCyana2.1.

At the end of the tutorial we explain Cryana new commands.

Files

We refer to original ParagneticCyana2.1 files.

New files:

crystaldata.f

getcrydip.f

Replaced files

findzerocoords.f
psegrad.f
pseviol.f

Modified files

copy.f
cyana.for
cyanadata.f
fcn.f
grad.f
readf.f
violst.f
viosta.f

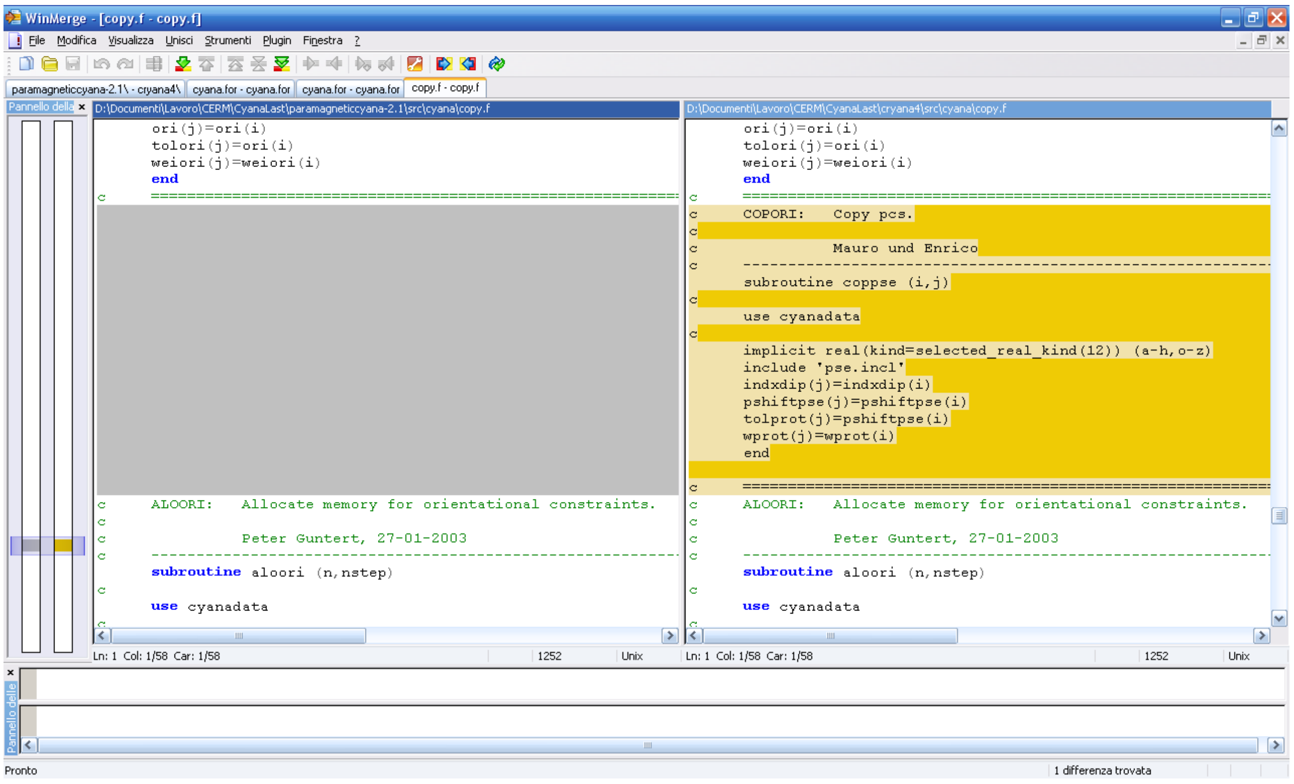
Details on modified files:

copy.f

add the subroutine:

```
c       ==================================================================
c       COPPSE:   Copy pcs.
c
c                 Mauro und Enrico
c       ------------------------------------------------------------------
        subroutine coppse (i,j)
c
        use cyanadata
c
        implicit real(kind=selected_real_kind(12)) (a-h,o-z)
        include 'pse.incl'
        indxdip(j)=indxdip(i)
        pshiftpse(j)=pshiftpse(i)
        tolprot(j)=pshiftpse(i)
        wprot(j)=wprot(i)
        end

c       ==================================================================
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\copy.f

```
        ori(j)=ori(i)
        tolori(j)=ori(i)
        weiori(j)=weiori(i)
        end
c       ==================================================================




















c       ALOORI:   Allocate memory for orientational constraints.
c
c                 Peter Guntert, 27-01-2003
c       ------------------------------------------------------------------
        subroutine aloori (n,nstep)
c
        use cyanadata
```

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D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\copy.f

```
        ori(j)=ori(i)
        tolori(j)=ori(i)
        weiori(j)=weiori(i)
        end
c       ==================================================================
c       COPORI:   Copy pcs.
c
c                 Mauro und Enrico
c       ------------------------------------------------------------------
        subroutine coppse (i,j)
c
        use cyanadata
c
        implicit real(kind=selected_real_kind(12)) (a-h,o-z)
        include 'pse.incl'
        indxdip(j)=indxdip(i)
        pshiftpse(j)=pshiftpse(i)
        tolprot(j)=pshiftpse(i)
        wprot(j)=wprot(i)
        end

c       ==================================================================
c       ALOORI:   Allocate memory for orientational constraints.
c
c                 Peter Guntert, 27-01-2003
c       ------------------------------------------------------------------
        subroutine aloori (n,nstep)
c
        use cyanadata
```

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1 differenza trovata

cyana.for

1) add

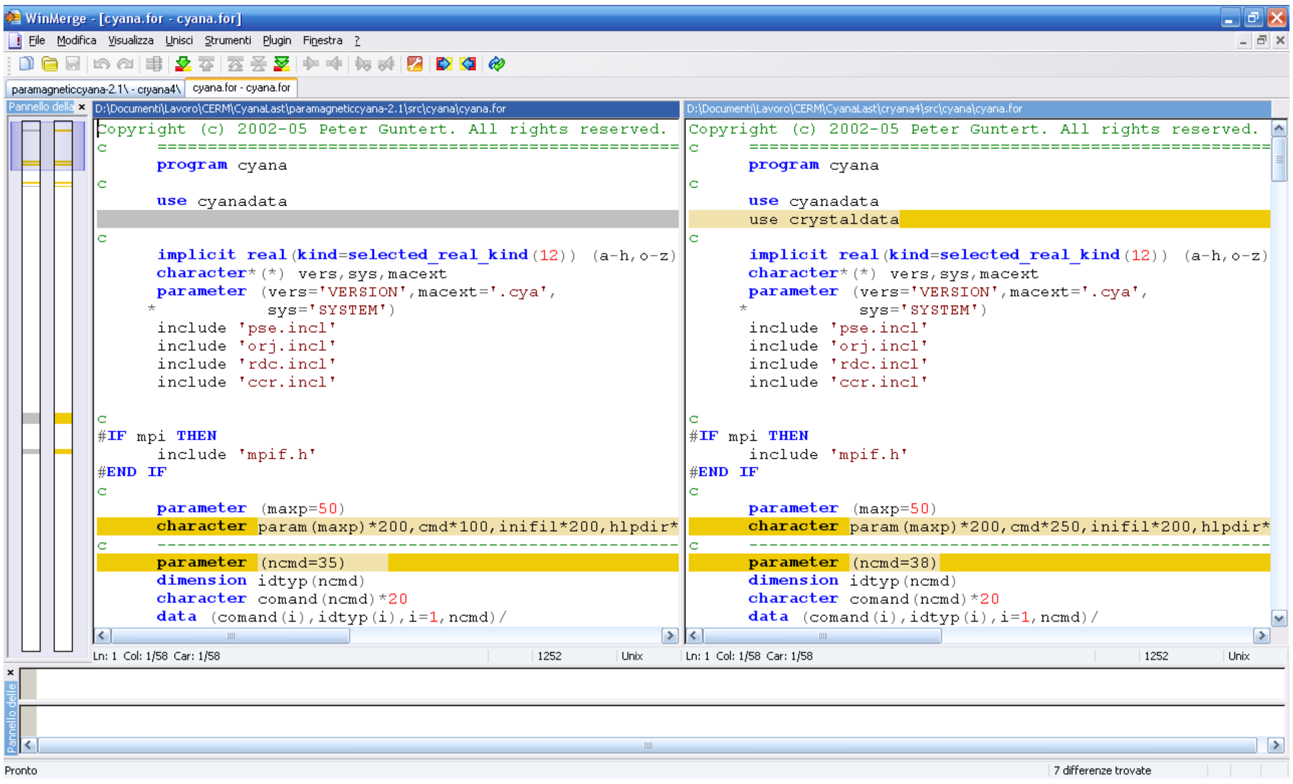
   ```
   use crystaldata
   ```

2) change

   `cmd*100` → `cmd*250`

3) add 3 parameters

   ```
   ncmd=38
   ```


WinMerge - [cyana.for - cyana.for]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\
cyana.for - cyana.for
Pannello della
Pannello delle

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\cyana.for

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c     ====================================================
      program cyana
c
      use cyanadata

c
      implicit real(kind=selected_real_kind(12))  (a-h,o-z)
      character*(*)  vers,sys,macext
      parameter  (vers='VERSION',macext='.cya',
     *            sys='SYSTEM')
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'


c
#IF mpi THEN
      include 'mpif.h'
#END IF
c
      parameter  (maxp=50)
      character param(maxp)*200,cmd*100,inifil*200,hlpdir*
c     ----------------------------------------------------
      parameter  (ncmd=35)
      dimension idtyp(ncmd)
      character comand(ncmd)*20
      data  (comand(i),idtyp(i),i=1,ncmd)/
```

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D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\cyana.for

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c     ====================================================
      program cyana
c
      use cyanadata
      use crystaldata
c
      implicit real(kind=selected_real_kind(12))  (a-h,o-z)
      character*(*)  vers,sys,macext
      parameter  (vers='VERSION',macext='.cya',
     *            sys='SYSTEM')
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'


c
#IF mpi THEN
      include 'mpif.h'
#END IF
c
      parameter  (maxp=50)
      character param(maxp)*200,cmd*250,inifil*200,hlpdir*
c     ----------------------------------------------------
      parameter  (ncmd=38)
      dimension idtyp(ncmd)
      character comand(ncmd)*20
      data  (comand(i),idtyp(i),i=1,ncmd)/
```

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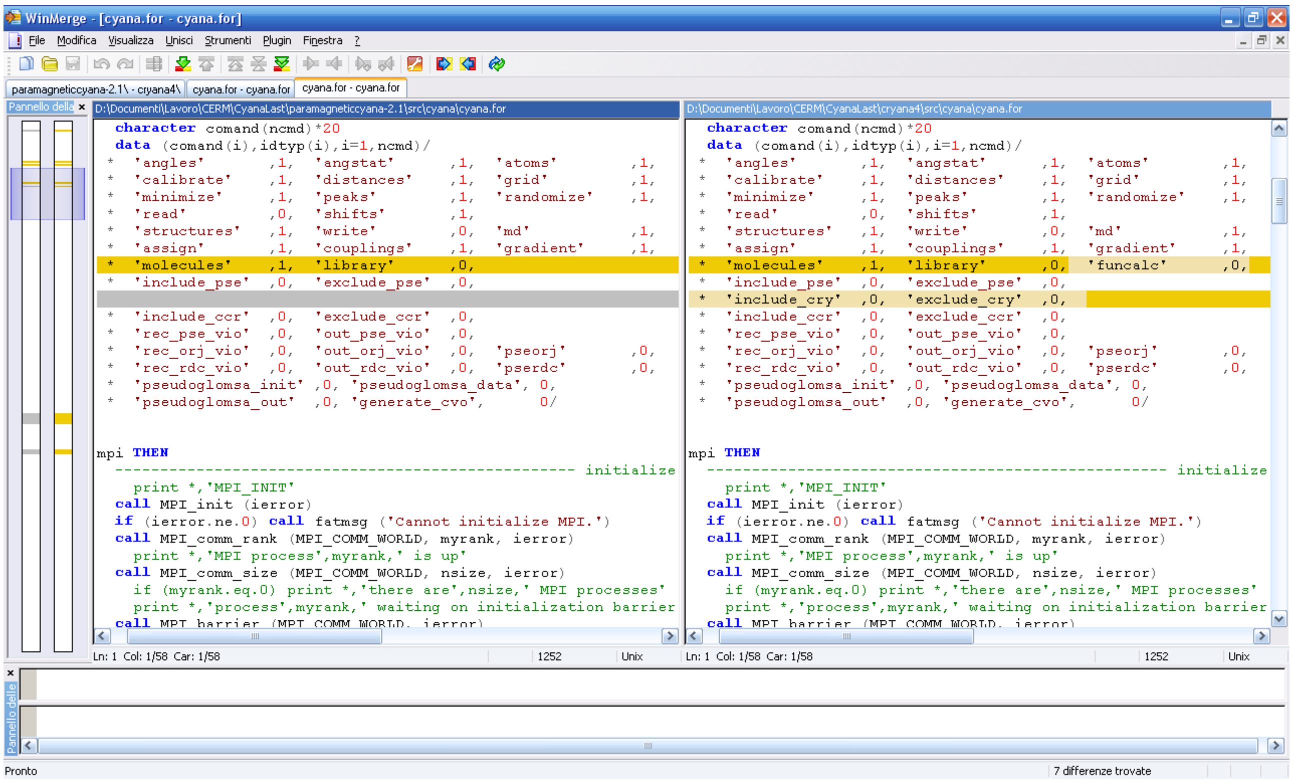
Pronto 7 differenze trovate

4) add

```
    'funcalc'      ,0,
 *  'include_cry'  ,0,  'exclude_cry'  ,0,
```


WinMerge - [cyana.for - cyana.for]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\
cyana.for - cyana.for
cyana.for - cyana.for
Pannello della
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D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\cyana.for

```
  character comand(ncmd)*20
  data  (comand(i),idtyp(i),i=1,ncmd)/
 *  'angles'        ,1,  'angstat'        ,1,  'atoms'          ,1,
 *  'calibrate'     ,1,  'distances'      ,1,  'grid'           ,1,
 *  'minimize'      ,1,  'peaks'          ,1,  'randomize'      ,1,
 *  'read'          ,0,  'shifts'         ,1,
 *  'structures'    ,1,  'write'          ,0,  'md'             ,1,
 *  'assign'        ,1,  'couplings'      ,1,  'gradient'       ,1,
 *  'molecules'     ,1,  'library'        ,0,
 *  'include_pse'  ,0,  'exclude_pse'   ,0,

 *  'include_ccr'  ,0,  'exclude_ccr'   ,0,
 *  'rec_pse_vio'  ,0,  'out_pse_vio'   ,0,
 *  'rec_orj_vio'  ,0,  'out_orj_vio'   ,0,  'pseorj'         ,0,
 *  'rec_rdc_vio'  ,0,  'out_rdc_vio'   ,0,  'pserdc'         ,0,
 *  'pseudoglomsa_init' ,0, 'pseudoglomsa_data', 0,
 *  'pseudoglomsa_out'  ,0, 'generate_cvo',      0/


mpi THEN
  ---------------------------------------------------- initialize
    print *,'MPI_INIT'
  call MPI_init (ierror)
  if (ierror.ne.0) call fatmsg ('Cannot initialize MPI.')
  call MPI_comm_rank (MPI_COMM_WORLD, myrank, ierror)
    print *,'MPI process',myrank,' is up'
  call MPI_comm_size (MPI_COMM_WORLD, nsize, ierror)
    if (myrank.eq.0) print *,'there are',nsize,' MPI processes'
    print *,'process',myrank,' waiting on initialization barrier
  call MPI_barrier (MPI_COMM_WORLD, ierror)
```

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D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\cyana.for

```
  character comand(ncmd)*20
  data  (comand(i),idtyp(i),i=1,ncmd)/
 *  'angles'        ,1,  'angstat'        ,1,  'atoms'          ,1,
 *  'calibrate'     ,1,  'distances'      ,1,  'grid'           ,1,
 *  'minimize'      ,1,  'peaks'          ,1,  'randomize'      ,1,
 *  'read'          ,0,  'shifts'         ,1,
 *  'structures'    ,1,  'write'          ,0,  'md'             ,1,
 *  'assign'        ,1,  'couplings'      ,1,  'gradient'       ,1,
 *  'molecules'     ,1,  'library'        ,0,  'funcalc'        ,0,
 *  'include_pse'  ,0,  'exclude_pse'   ,0,
 *  'include_cry'  ,0,  'exclude_cry'   ,0,
 *  'include_ccr'  ,0,  'exclude_ccr'   ,0,
 *  'rec_pse_vio'  ,0,  'out_pse_vio'   ,0,
 *  'rec_orj_vio'  ,0,  'out_orj_vio'   ,0,  'pseorj'         ,0,
 *  'rec_rdc_vio'  ,0,  'out_rdc_vio'   ,0,  'pserdc'         ,0,
 *  'pseudoglomsa_init' ,0, 'pseudoglomsa_data', 0,
 *  'pseudoglomsa_out'  ,0, 'generate_cvo',      0/


mpi THEN
  ---------------------------------------------------- initialize
    print *,'MPI_INIT'
  call MPI_init (ierror)
  if (ierror.ne.0) call fatmsg ('Cannot initialize MPI.')
  call MPI_comm_rank (MPI_COMM_WORLD, myrank, ierror)
    print *,'MPI process',myrank,' is up'
  call MPI_comm_size (MPI_COMM_WORLD, nsize, ierror)
    if (myrank.eq.0) print *,'there are',nsize,' MPI processes'
    print *,'process',myrank,' waiting on initialization barrier
  call MPI_barrier (MPI_COMM_WORLD, ierror)
```

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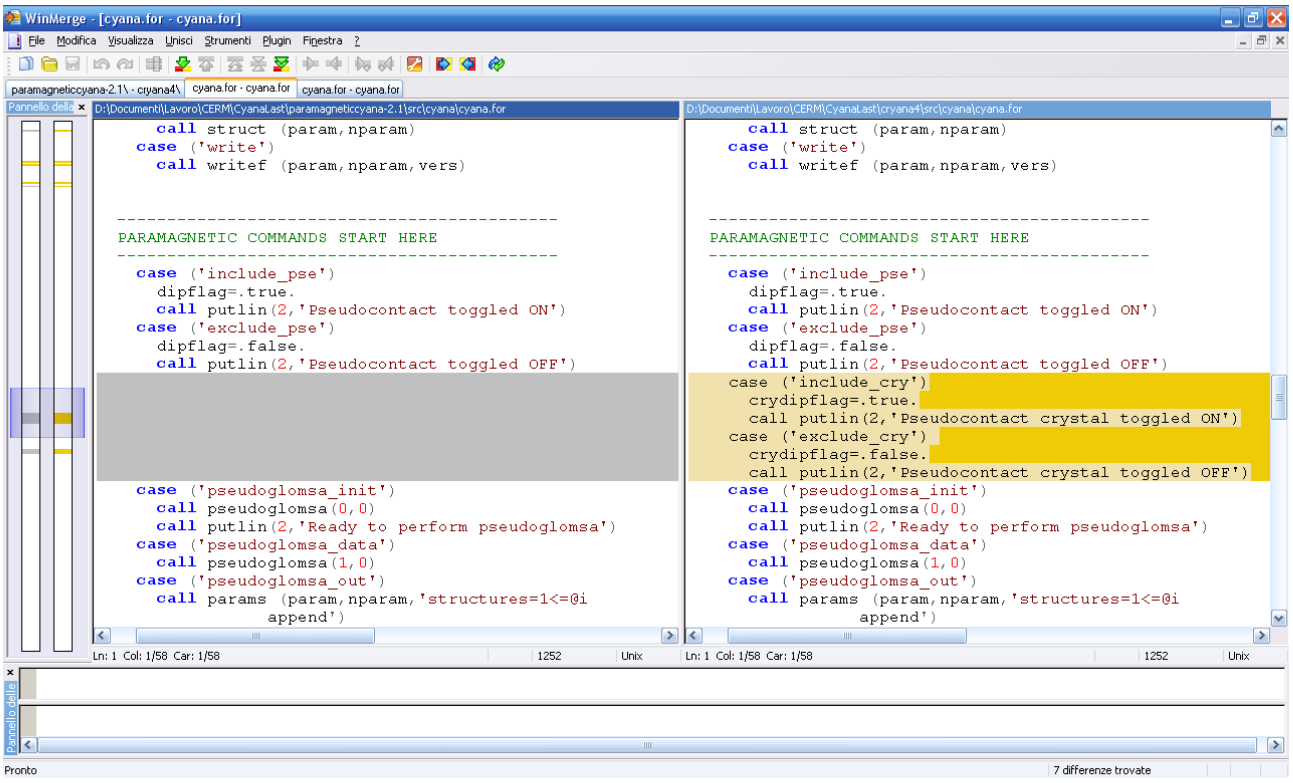
Pronto 7 differenze trovate

5) add

```
case ('include_cry')
     crydipflag=.true.
     call putlin(2,'Pseudocontact crystal toggled ON')
 case ('exclude_cry')
     crydipflag=.false.
     call putlin(2,'Pseudocontact crystal toggled OFF')
```


WinMerge - [cyana.for - cyana.for]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\
cyana.for - cyana.for
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Pannello della
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D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\cyana.for

```
        call struct  (param,nparam)
     case ('write')
        call writef  (param,nparam,vers)


  --------------------------------------------
  PARAMAGNETIC COMMANDS START HERE
  --------------------------------------------
     case ('include_pse')
        dipflag=.true.
        call putlin(2,'Pseudocontact toggled ON')
     case ('exclude_pse')
        dipflag=.false.
        call putlin(2,'Pseudocontact toggled OFF')






     case ('pseudoglomsa_init')
        call pseudoglomsa(0,0)
        call putlin(2,'Ready to perform pseudoglomsa')
     case ('pseudoglomsa_data')
        call pseudoglomsa(1,0)
     case ('pseudoglomsa_out')
        call params  (param,nparam,'structures=1<=@i
                     append')
```

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D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\cyana.for

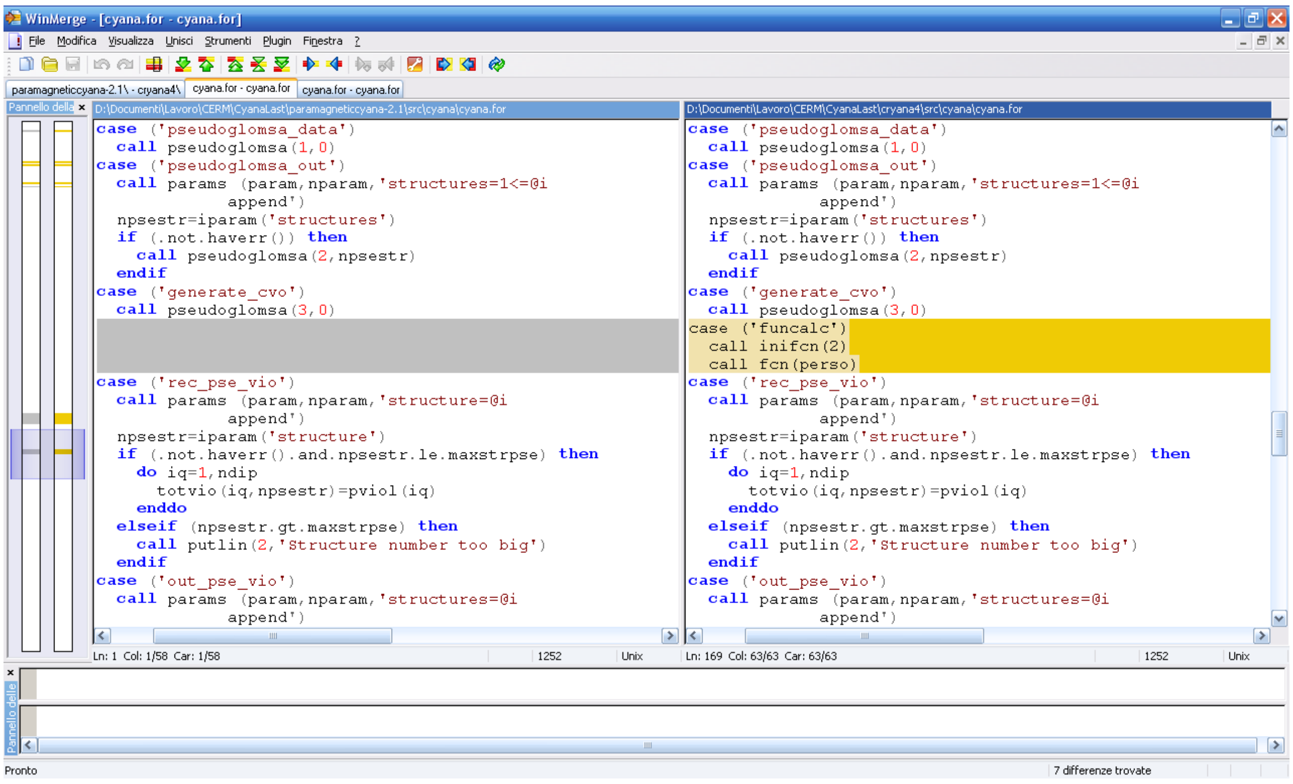
```
        call struct  (param,nparam)
     case ('write')
        call writef  (param,nparam,vers)


  --------------------------------------------
  PARAMAGNETIC COMMANDS START HERE
  --------------------------------------------
     case ('include_pse')
        dipflag=.true.
        call putlin(2,'Pseudocontact toggled ON')
     case ('exclude_pse')
        dipflag=.false.
        call putlin(2,'Pseudocontact toggled OFF')
     case ('include_cry')
        crydipflag=.true.
        call putlin(2,'Pseudocontact crystal toggled ON')
     case ('exclude_cry')
        crydipflag=.false.
        call putlin(2,'Pseudocontact crystal toggled OFF')
     case ('pseudoglomsa_init')
        call pseudoglomsa(0,0)
        call putlin(2,'Ready to perform pseudoglomsa')
     case ('pseudoglomsa_data')
        call pseudoglomsa(1,0)
     case ('pseudoglomsa_out')
        call params  (param,nparam,'structures=1<=@i
                     append')
```

Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

Pronto 7 differenze trovate

6) add

```
 case ('funcalc')
     call inifcn(2)
     call fcn(perso)
```


WinMerge - [cyana.for - cyana.for]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\cyana.for

```
case ('pseudoglomsa_data')
  call pseudoglomsa(1,0)
case ('pseudoglomsa_out')
  call params (param,nparam,'structures=1<=@i
                append')
  npsestr=iparam('structures')
  if (.not.haverr()) then
    call pseudoglomsa(2,npsestr)
  endif
case ('generate_cvo')
  call pseudoglomsa(3,0)



case ('rec_pse_vio')
  call params (param,nparam,'structure=@i
                append')
  npsestr=iparam('structure')
  if (.not.haverr().and.npsestr.le.maxstrpse) then
    do iq=1,ndip
      totvio(iq,npsestr)=pviol(iq)
    enddo
  elseif (npsestr.gt.maxstrpse) then
    call putlin(2,'Structure number too big')
  endif
case ('out_pse_vio')
  call params (param,nparam,'structures=@i
                append')
```

Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\cyana.for

```
case ('pseudoglomsa_data')
  call pseudoglomsa(1,0)
case ('pseudoglomsa_out')
  call params (param,nparam,'structures=1<=@i
                append')
  npsestr=iparam('structures')
  if (.not.haverr()) then
    call pseudoglomsa(2,npsestr)
  endif
case ('generate_cvo')
  call pseudoglomsa(3,0)
case ('funcalc')
  call inifcn(2)
  call fcn(perso)
case ('rec_pse_vio')
  call params (param,nparam,'structure=@i
                append')
  npsestr=iparam('structure')
  if (.not.haverr().and.npsestr.le.maxstrpse) then
    do iq=1,ndip
      totvio(iq,npsestr)=pviol(iq)
    enddo
  elseif (npsestr.gt.maxstrpse) then
    call putlin(2,'Structure number too big')
  endif
case ('out_pse_vio')
  call params (param,nparam,'structures=@i
                append')
```

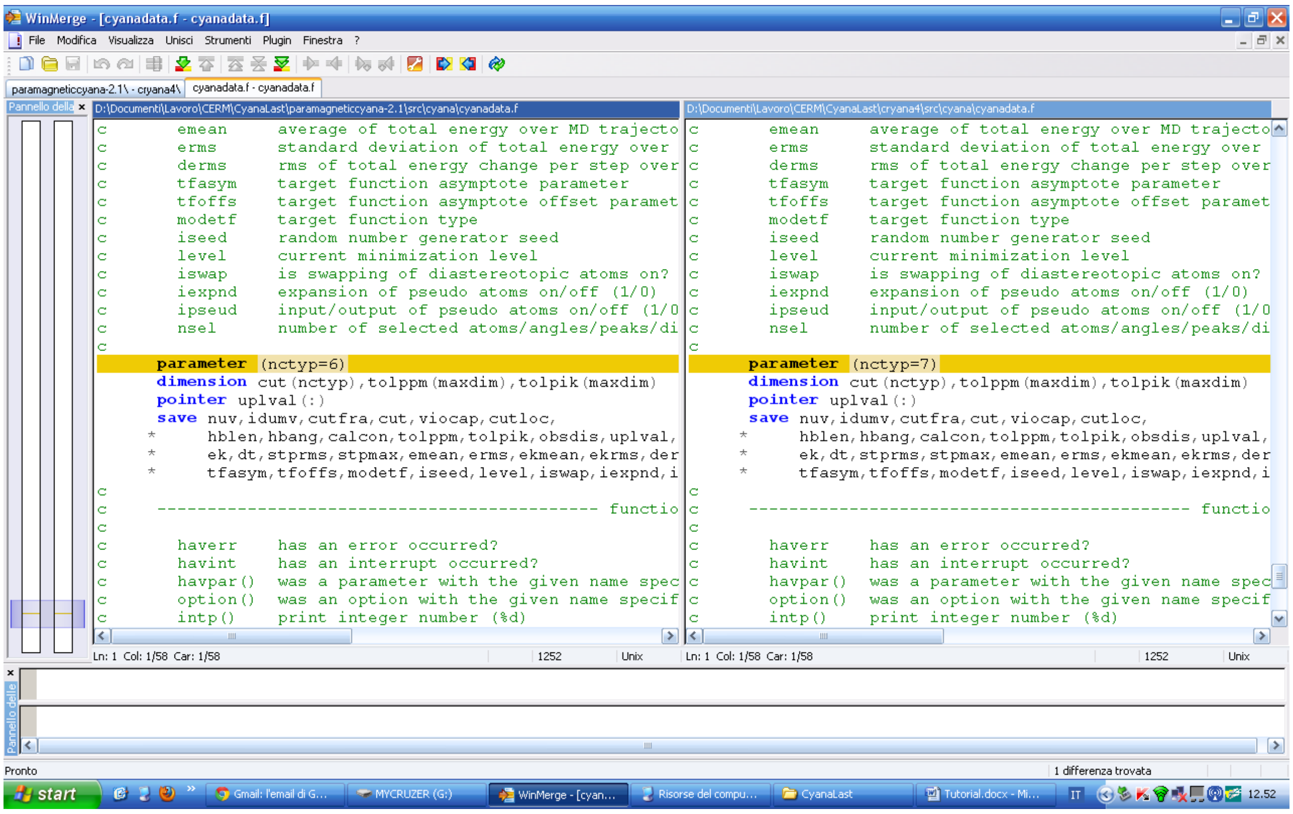
Ln: 169 Col: 63/63 Car: 63/63 1252 Unix

Pronto 7 differenze trovate

cyanadata.f

1) change

```
nctyp=6    →    nctyp=7
```


WinMerge - [cyanadata.f - cyanadata.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\cyanadata.f

```
c        emean      average of total energy over MD trajecto
c        erms       standard deviation of total energy over
c        derms      rms of total energy change per step over
c        tfasym     target function asymptote parameter
c        tfoffs     target function asymptote offset paramet
c        modetf     target function type
c        iseed      random number generator seed
c        level      current minimization level
c        iswap      is swapping of diastereotopic atoms on?
c        iexpnd     expansion of pseudo atoms on/off (1/0)
c        ipseud     input/output of pseudo atoms on/off (1/0
c        nsel       number of selected atoms/angles/peaks/di
c
      parameter (nctyp=6)
      dimension cut(nctyp),tolppm(maxdim),tolpik(maxdim)
      pointer uplval(:)
      save nuv,iduмv,cutfra,cut,viocap,cutloc,
     *     hblen,hbang,calcon,tolppm,tolpik,obsdis,uplval,
     *     ek,dt,stprms,stpmax,emean,erms,ekmean,ekrms,der
     *     tfasym,tfoffs,modetf,iseed,level,iswap,iexpnd,i
c
c     --------------------------------------------- functio
c
c        haverr     has an error occurred?
c        havint     has an interrupt occurred?
c        havpar()   was a parameter with the given name spec
c        option()   was an option with the given name specif
c        intp()     print integer number (%d)
```

Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\cyanadata.f

```
c        emean      average of total energy over MD trajecto
c        erms       standard deviation of total energy over
c        derms      rms of total energy change per step over
c        tfasym     target function asymptote parameter
c        tfoffs     target function asymptote offset paramet
c        modetf     target function type
c        iseed      random number generator seed
c        level      current minimization level
c        iswap      is swapping of diastereotopic atoms on?
c        iexpnd     expansion of pseudo atoms on/off (1/0)
c        ipseud     input/output of pseudo atoms on/off (1/0
c        nsel       number of selected atoms/angles/peaks/di
c
      parameter (nctyp=7)
      dimension cut(nctyp),tolppm(maxdim),tolpik(maxdim)
      pointer uplval(:)
      save nuv,idumv,cutfra,cut,viocap,cutloc,
     *     hblen,hbang,calcon,tolppm,tolpik,obsdis,uplval,
     *     ek,dt,stprms,stpmax,emean,erms,ekmean,ekrms,der
     *     tfasym,tfoffs,modetf,iseed,level,iswap,iexpnd,i
c
c     --------------------------------------------- functio
c
c        haverr     has an error occurred?
c        havint     has an interrupt occurred?
c        havpar()   was a parameter with the given name spec
c        option()   was an option with the given name specif
c        intp()     print integer number (%d)
```

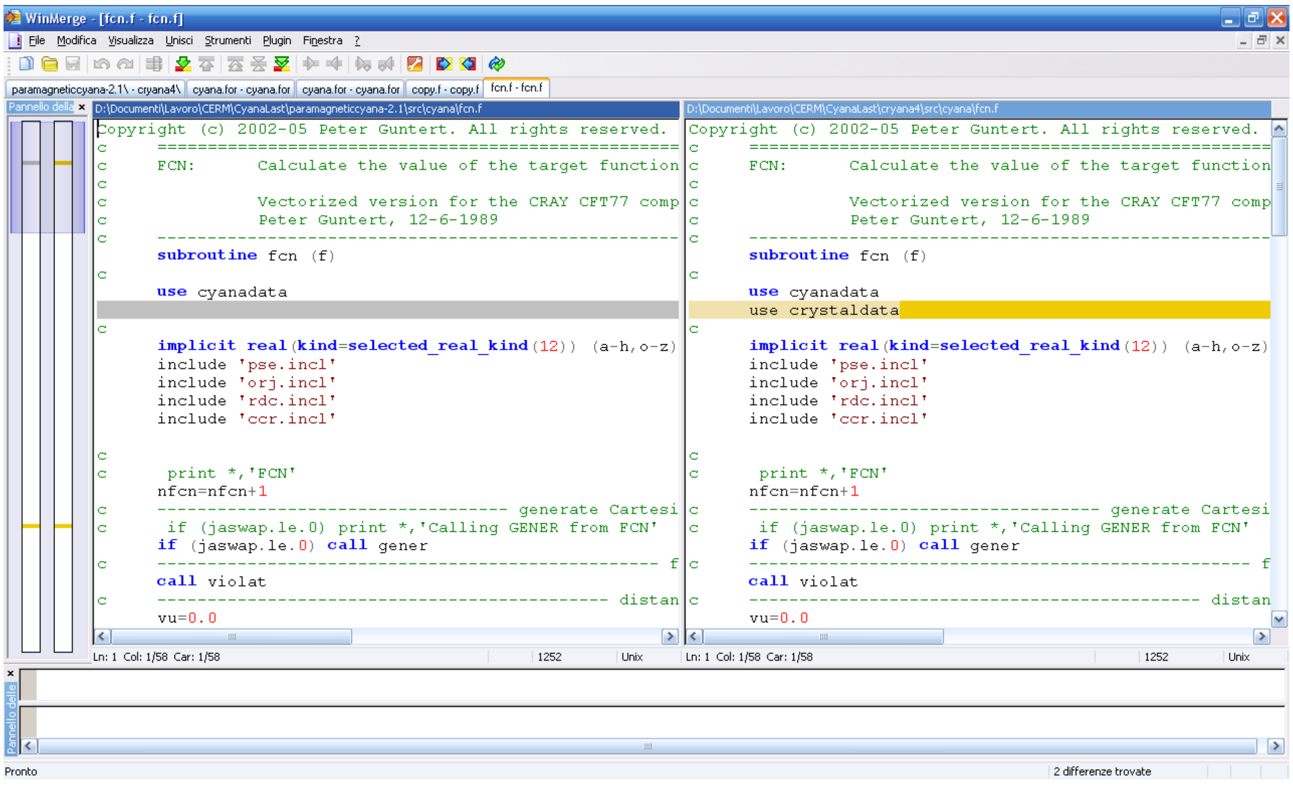
Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

Pronto 1 differenza trovata

fcn.f

1) add

```
use crystaldata
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\fcn.f

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c ======================================================
c      FCN:      Calculate the value of the target function
c
c                Vectorized version for the CRAY CFT77 comp
c                Peter Guntert, 12-6-1989
c      ----------------------------------------------------
       subroutine fcn (f)
c
       use cyanadata

c
       implicit real(kind=selected_real_kind(12)) (a-h,o-z)
       include 'pse.incl'
       include 'orj.incl'
       include 'rdc.incl'
       include 'ccr.incl'

c
c       print *,'FCN'
       nfcn=nfcn+1
c      ----------------------------------- generate Cartesi
c       if (jaswap.le.0) print *,'Calling GENER from FCN'
       if (jaswap.le.0) call gener
c      ---------------------------------------------------- f
       call violat
c      ----------------------------------------------- distan
       vu=0.0
```

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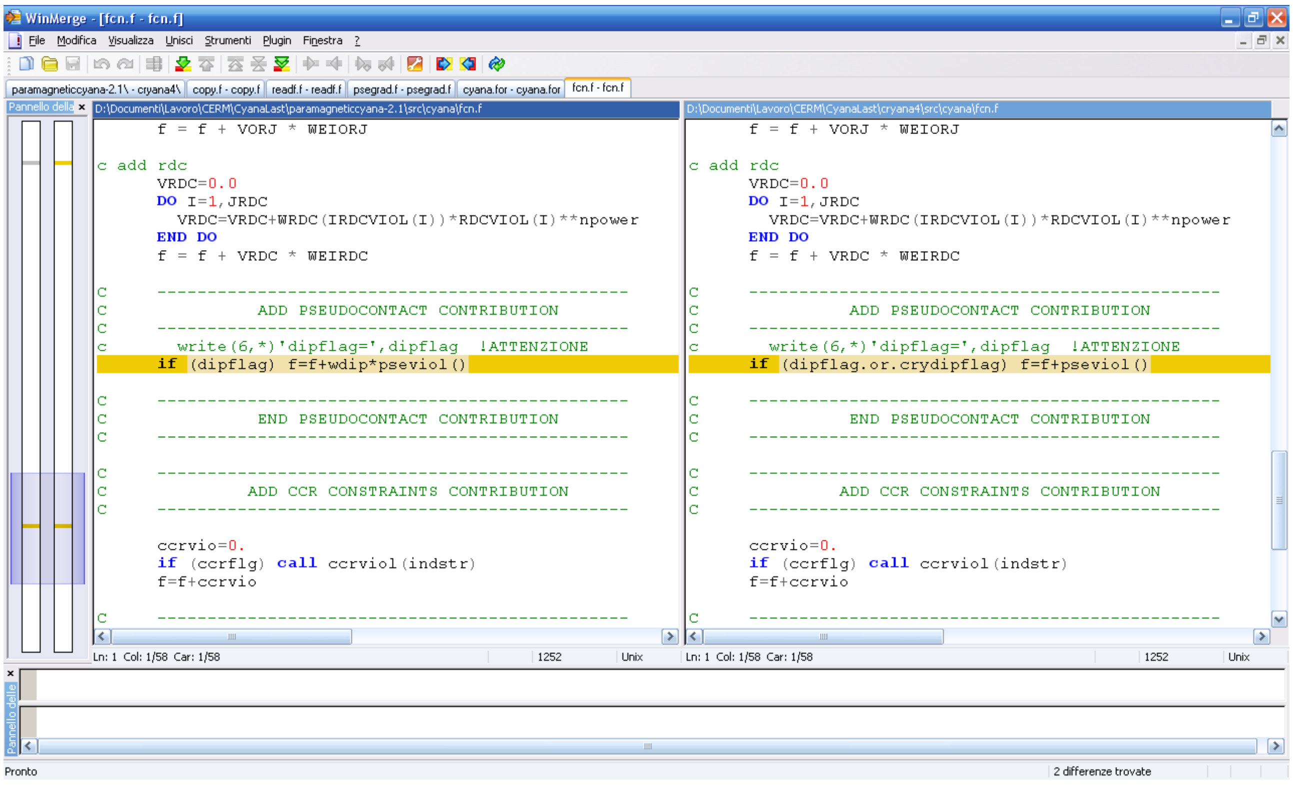
D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\fcn.f

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c ======================================================
c      FCN:      Calculate the value of the target function
c
c                Vectorized version for the CRAY CFT77 comp
c                Peter Guntert, 12-6-1989
c      ----------------------------------------------------
       subroutine fcn (f)
c
       use cyanadata
       use crystaldata
c
       implicit real(kind=selected_real_kind(12)) (a-h,o-z)
       include 'pse.incl'
       include 'orj.incl'
       include 'rdc.incl'
       include 'ccr.incl'

c
c       print *,'FCN'
       nfcn=nfcn+1
c      ----------------------------------- generate Cartesi
c       if (jaswap.le.0) print *,'Calling GENER from FCN'
       if (jaswap.le.0) call gener
c      ---------------------------------------------------- f
       call violat
c      ----------------------------------------------- distan
       vu=0.0
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

2) change

```
if (dipflag) f=f+wdip*pseviol()   →   if (dipflag.or.crydipflag) f=f+pseviol()
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\fcn.f

```
       f = f + VORJ * WEIORJ

c add rdc
       VRDC=0.0
       DO I=1,JRDC
         VRDC=VRDC+WRDC(IRDCVIOL(I))*RDCVIOL(I)**npower
       END DO
       f = f + VRDC * WEIRDC

C      ----------------------------------------------
C                ADD PSEUDOCONTACT CONTRIBUTION
C      ----------------------------------------------
c        write(6,*)'dipflag=',dipflag  !ATTENZIONE
       if (dipflag) f=f+wdip*pseviol()

C      ----------------------------------------------
C                END PSEUDOCONTACT CONTRIBUTION
C      ----------------------------------------------

C      ----------------------------------------------
C               ADD CCR CONSTRAINTS CONTRIBUTION
C      ----------------------------------------------

       ccrvio=0.
       if (ccrflg) call ccrviol(indstr)
       f=f+ccrvio

C      ----------------------------------------------
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\fcn.f

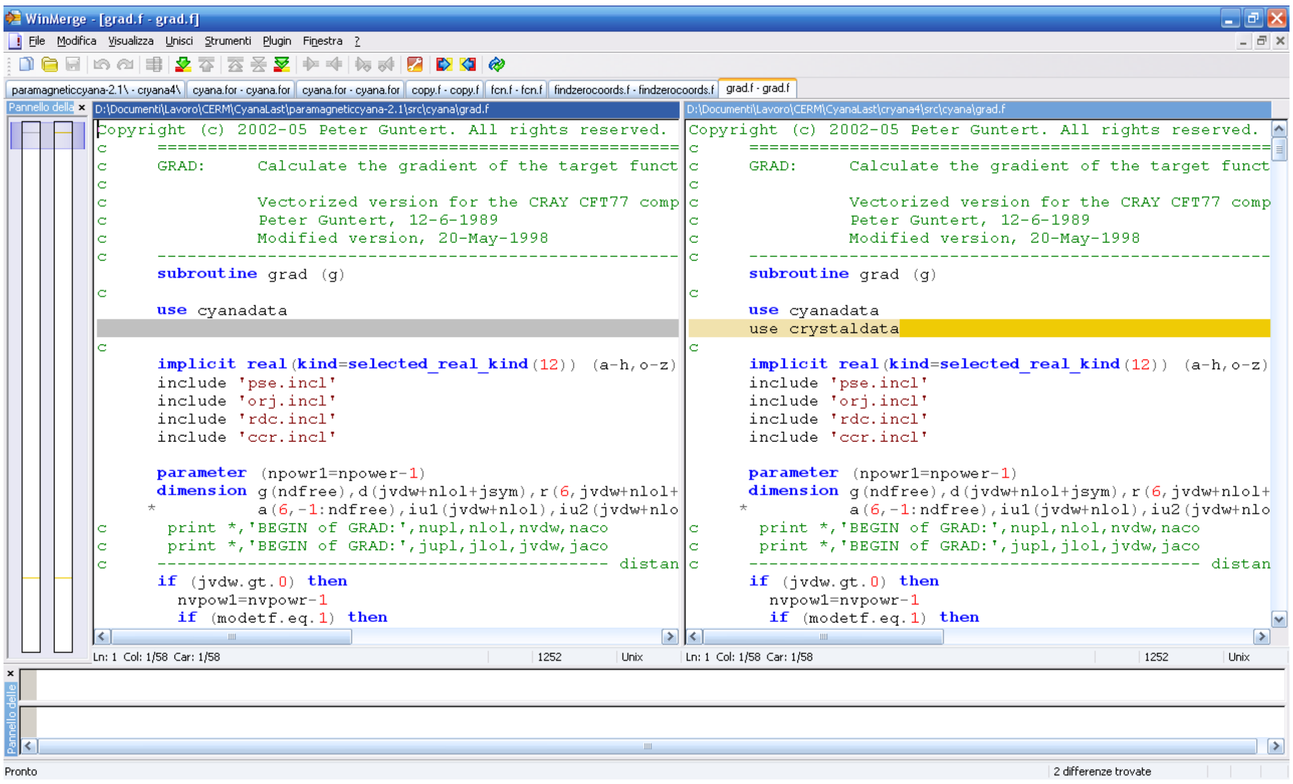
```
       f = f + VORJ * WEIORJ

c add rdc
       VRDC=0.0
       DO I=1,JRDC
         VRDC=VRDC+WRDC(IRDCVIOL(I))*RDCVIOL(I)**npower
       END DO
       f = f + VRDC * WEIRDC

C      ----------------------------------------------
C                ADD PSEUDOCONTACT CONTRIBUTION
C      ----------------------------------------------
c        write(6,*)'dipflag=',dipflag  !ATTENZIONE
       if (dipflag.or.crydipflag) f=f+pseviol()

C      ----------------------------------------------
C                END PSEUDOCONTACT CONTRIBUTION
C      ----------------------------------------------

C      ----------------------------------------------
C               ADD CCR CONSTRAINTS CONTRIBUTION
C      ----------------------------------------------

       ccrvio=0.
       if (ccrflg) call ccrviol(indstr)
       f=f+ccrvio

C      ----------------------------------------------
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

grad.f

1) add

```
use crystaldata
```


WinMerge - [grad.f - grad.f]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\
cyana.for - cyana.for
cyana.for - cyana.for
copy.f - copy.f
fcn.f - fcn.f
findzerocoords.f - findzerocoords.f
grad.f - grad.f
Pannello della
Pannello delle

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\grad.f

```
Copyright  (c) 2002-05 Peter Guntert. All rights reserved.
c     ========================================================
c     GRAD:     Calculate the gradient of the target funct
c
c               Vectorized version for the CRAY CFT77 comp
c               Peter Guntert, 12-6-1989
c               Modified version, 20-May-1998
c     --------------------------------------------------------
      subroutine grad (g)
c
      use cyanadata

c
      implicit real(kind=selected_real_kind(12)) (a-h,o-z)
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'

      parameter (npowr1=npower-1)
      dimension g(ndfree),d(jvdw+nlol+jsym),r(6,jvdw+nlol+
     *          a(6,-1:ndfree),iu1(jvdw+nlol),iu2(jvdw+nlo
c      print *,'BEGIN of GRAD:',nupl,nlol,nvdw,naco
c      print *,'BEGIN of GRAD:',jupl,jlol,jvdw,jaco
c     -------------------------------------------- distan
      if (jvdw.gt.0) then
        nvpowl=nvpowr-1
        if (modetf.eq.1) then
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\grad.f

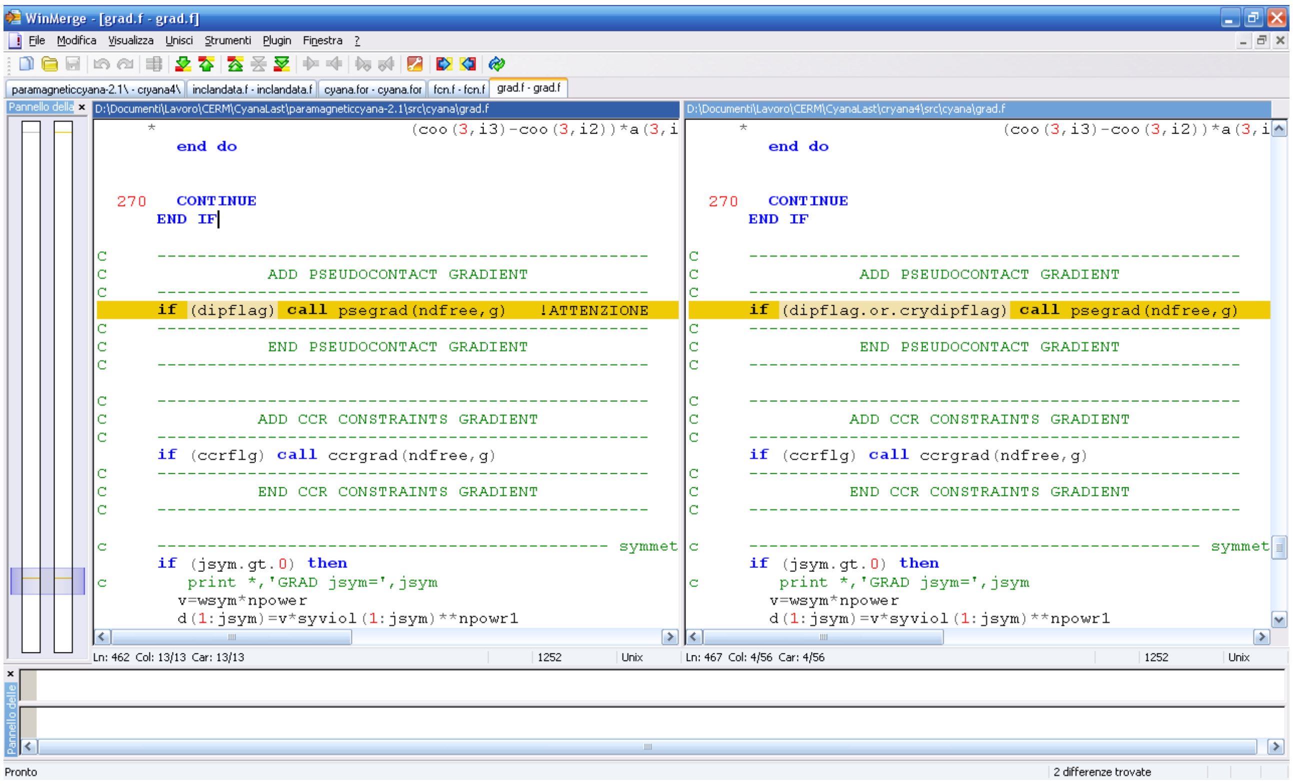
```
Copyright  (c) 2002-05 Peter Guntert. All rights reserved.
c     ========================================================
c     GRAD:     Calculate the gradient of the target funct
c
c               Vectorized version for the CRAY CFT77 comp
c               Peter Guntert, 12-6-1989
c               Modified version, 20-May-1998
c     --------------------------------------------------------
      subroutine grad (g)
c
      use cyanadata
      use crystaldata
c
      implicit real(kind=selected_real_kind(12)) (a-h,o-z)
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'

      parameter (npowr1=npower-1)
      dimension g(ndfree),d(jvdw+nlol+jsym),r(6,jvdw+nlol+
     *          a(6,-1:ndfree),iu1(jvdw+nlol),iu2(jvdw+nlo
c      print *,'BEGIN of GRAD:',nupl,nlol,nvdw,naco
c      print *,'BEGIN of GRAD:',jupl,jlol,jvdw,jaco
c     -------------------------------------------- distan
      if (jvdw.gt.0) then
        nvpowl=nvpowr-1
        if (modetf.eq.1) then
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

Pronto   2 differenze trovate

2) change

```
    if (dipflag) call psegrad(ndfree,g)   →   if (dipflag.or.crydipflag) call psegrad(ndfree,g)
```


WinMerge - [grad.f - grad.f]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\
inclandata.f - inclandata.f
cyana.for - cyana.for
fcn.f - fcn.f
grad.f - grad.f
Pannello della
Pannello delle

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\grad.f

```
     *                                 (coo(3,i3)-coo(3,i2))*a(3,i
        end do


 270    CONTINUE
      END IF

c     ------------------------------------------------
c                ADD PSEUDOCONTACT GRADIENT
c     ------------------------------------------------
      if (dipflag) call psegrad(ndfree,g)    !ATTENZIONE
c     ------------------------------------------------
c                END PSEUDOCONTACT GRADIENT
c     ------------------------------------------------

c     ------------------------------------------------
c               ADD CCR CONSTRAINTS GRADIENT
c     ------------------------------------------------
      if (ccrflg) call ccrgrad(ndfree,g)
c     ------------------------------------------------
c               END CCR CONSTRAINTS GRADIENT
c     ------------------------------------------------

c     -------------------------------------------- symmet
      if (jsym.gt.0) then
c        print *,'GRAD jsym=',jsym
        v=wsym*npower
        d(1:jsym)=v*syviol(1:jsym)**npowr1
```

Ln: 462 Col: 13/13 Car: 13/13   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\grad.f

```
     *                                 (coo(3,i3)-coo(3,i2))*a(3,i
        end do


 270    CONTINUE
      END IF

c     ------------------------------------------------
c                ADD PSEUDOCONTACT GRADIENT
c     ------------------------------------------------
      if (dipflag.or.crydipflag) call psegrad(ndfree,g)
c     ------------------------------------------------
c                END PSEUDOCONTACT GRADIENT
c     ------------------------------------------------

c     ------------------------------------------------
c               ADD CCR CONSTRAINTS GRADIENT
c     ------------------------------------------------
      if (ccrflg) call ccrgrad(ndfree,g)
c     ------------------------------------------------
c               END CCR CONSTRAINTS GRADIENT
c     ------------------------------------------------

c     -------------------------------------------- symmet
      if (jsym.gt.0) then
c        print *,'GRAD jsym=',jsym
        v=wsym*npower
        d(1:jsym)=v*syviol(1:jsym)**npowr1
```

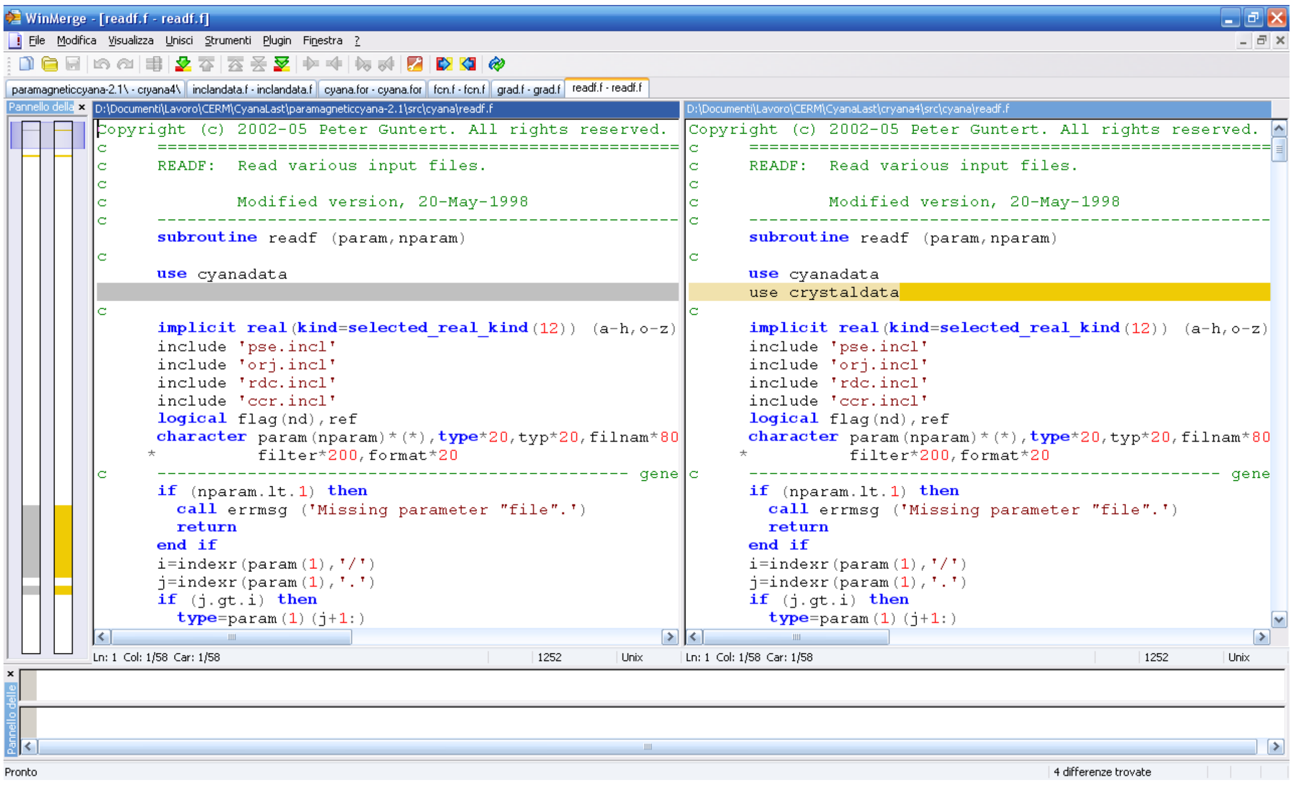
Ln: 467 Col: 4/56 Car: 4/56   1252   Unix

Pronto   2 differenze trovate

readf.f

1) add

```
    use crystaldata
```


WinMerge - [readf.f - readf.f]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\ | inclandata.f - inclandata.f | cyana.for - cyana.for | fcn.f - fcn.f | grad.f - grad.f | readf.f - readf.f
Pannello delle

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\readf.f

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c     ==========================================================
c     READF:  Read various input files.
c
c             Modified version, 20-May-1998
c     ----------------------------------------------------------
      subroutine readf (param,nparam)
c
      use cyanadata

c
      implicit real(kind=selected_real_kind(12)) (a-h,o-z)
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'
      logical flag(nd),ref
      character param(nparam)*(*),type*20,typ*20,filnam*80
     *          filter*200,format*20
c     ------------------------------------------------- gene
      if (nparam.lt.1) then
        call errmsg ('Missing parameter "file".')
        return
      end if
      i=indexr(param(1),'/')
      j=indexr(param(1),'.')
      if (j.gt.i) then
        type=param(1)(j+1:)
```

Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

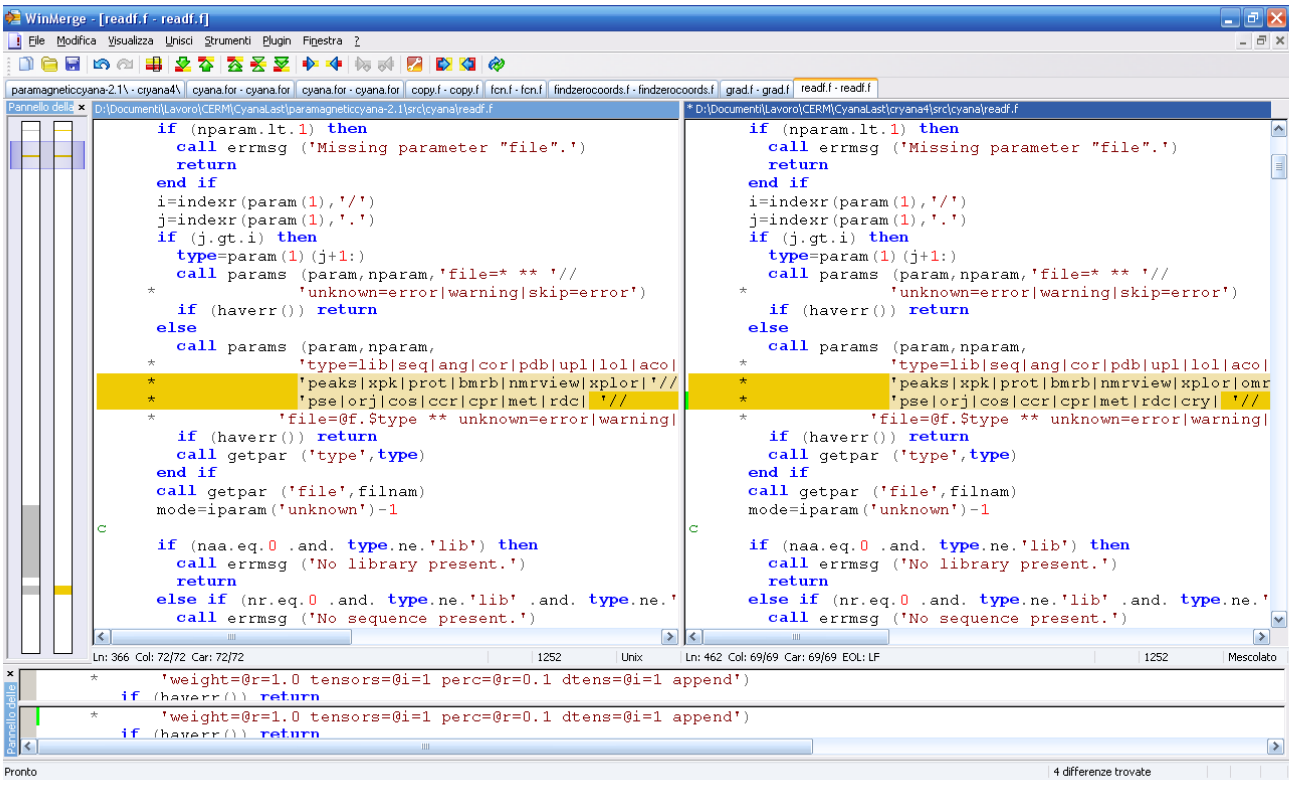
D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\readf.f

```
Copyright (c) 2002-05 Peter Guntert. All rights reserved.
c     ==========================================================
c     READF:  Read various input files.
c
c             Modified version, 20-May-1998
c     ----------------------------------------------------------
      subroutine readf (param,nparam)
c
      use cyanadata
      use crystaldata
c
      implicit real(kind=selected_real_kind(12)) (a-h,o-z)
      include 'pse.incl'
      include 'orj.incl'
      include 'rdc.incl'
      include 'ccr.incl'
      logical flag(nd),ref
      character param(nparam)*(*),type*20,typ*20,filnam*80
     *          filter*200,format*20
c     ------------------------------------------------- gene
      if (nparam.lt.1) then
        call errmsg ('Missing parameter "file".')
        return
      end if
      i=indexr(param(1),'/')
      j=indexr(param(1),'.')
      if (j.gt.i) then
        type=param(1)(j+1:)
```

Ln: 1 Col: 1/58 Car: 1/58 1252 Unix

Pronto 4 differenze trovate

2) add `omr` and `cry`


WinMerge - [readf.f - readf.f]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\ | cyana.for - cyana.for | cyana.for - cyana.for | copy.f - copy.f | fcn.f - fcn.f | findzerocoords.f - findzerocoords.f | grad.f - grad.f | readf.f - readf.f
Pannello delle

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\readf.f

```
      if (nparam.lt.1) then
        call errmsg ('Missing parameter "file".')
        return
      end if
      i=indexr(param(1),'/')
      j=indexr(param(1),'.')
      if (j.gt.i) then
        type=param(1)(j+1:)
        call params (param,nparam,'file=* ** '//
     *               'unknown=error|warning|skip=error')
        if (haverr()) return
      else
        call params (param,nparam,
     *               'type=lib|seq|ang|cor|pdb|upl|lol|aco|
     *               'peaks|xpk|prot|bmrb|nmrview|xplor|'//
     *               'pse|orj|cos|ccr|cpr|met|rdc|  '//
     *             'file=@f.$type ** unknown=error|warning|
        if (haverr()) return
        call getpar ('type',type)
      end if
      call getpar ('file',filnam)
      mode=iparam('unknown')-1
c
      if (naa.eq.0 .and. type.ne.'lib') then
        call errmsg ('No library present.')
        return
      else if (nr.eq.0 .and. type.ne.'lib' .and. type.ne.'
        call errmsg ('No sequence present.')
```

Ln: 366 Col: 72/72 Car: 72/72 1252 Unix

* D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\readf.f

```
      if (nparam.lt.1) then
        call errmsg ('Missing parameter "file".')
        return
      end if
      i=indexr(param(1),'/')
      j=indexr(param(1),'.')
      if (j.gt.i) then
        type=param(1)(j+1:)
        call params (param,nparam,'file=* ** '//
     *               'unknown=error|warning|skip=error')
        if (haverr()) return
      else
        call params (param,nparam,
     *               'type=lib|seq|ang|cor|pdb|upl|lol|aco|
     *               'peaks|xpk|prot|bmrb|nmrview|xplor|omr
     *               'pse|orj|cos|ccr|cpr|met|rdc|cry|  '//
     *             'file=@f.$type ** unknown=error|warning|
        if (haverr()) return
        call getpar ('type',type)
      end if
      call getpar ('file',filnam)
      mode=iparam('unknown')-1
c
      if (naa.eq.0 .and. type.ne.'lib') then
        call errmsg ('No library present.')
        return
      else if (nr.eq.0 .and. type.ne.'lib' .and. type.ne.'
        call errmsg ('No sequence present.')
```

Ln: 462 Col: 69/69 Car: 69/69 EOL: LF 1252 Mescolato

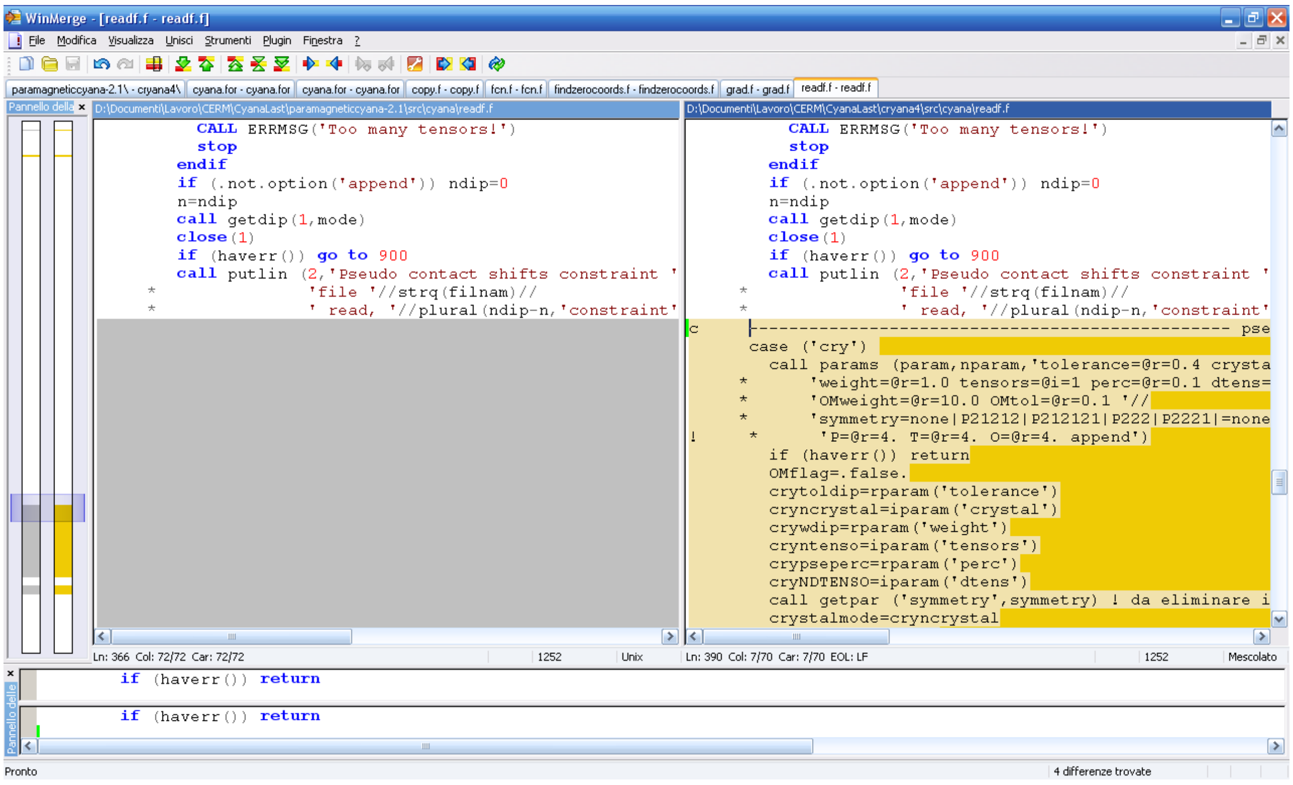
```
     *       'weight=@r=1.0 tensors=@i=1 perc=@r=0.1 dtens=@i=1 append')
        if (haverr()) return
```

```
     *       'weight=@r=1.0 tensors=@i=1 perc=@r=0.1 dtens=@i=1 append')
        if (haverr()) return
```

Pronto 4 differenze trovate

3) add `cry` case

```
c      ------------------------------------------------ pseudo
       case ('cry')
         call params (param,nparam,'tolerance=@r=0.4 crystal=@i=1 '//
     *        'weight=@r=1.0 tensors=@i=1 perc=@r=0.1 dtens=@i=1 '//
     *        'OMweight=@r=10.0 OMtol=@r=0.1 '//
*      'celldimx=@r=0.0 celldimy=@r=0.0 celldimz=@r=0.0 '//
*      'symmetry=none|P21212|P212121|P222|P2221|=none append')
   if (haverr()) return
   OMflag=.false.
   crytoldip=rparam('tolerance')
   cryncrystal=iparam('crystal')
   crywdip=rparam('weight')
   cryntenso=iparam('tensors')
   crypseperc=rparam('perc')
   cryNDTENSO=iparam('dtens')
   cellDim(1)=rparam('celldimx')
   cellDim(2)=rparam('celldimy')
   cellDim(3)=rparam('celldimz')
   call getpar ('symmetry',symmetry)
   crystalmode=cryncrystal
  if (cellDim(1).eq.0.0.or.cellDim(2).eq.0.0.or.cellDim(3).eq.0.0)
*    then
     CALL ERRMSG('Please insert crystal cell dimensions '//
*                                'celldimx, celldimy, celldimz')
     stop
  end if
   select case (cryncrystal)
   case (0)
          SolidState=.false.
   case (1)
          SolidState=.true.
           call putlin (2,'Crystal mode')
          !inizializzazione matrici di rotazione per pcs con stato solido
          call initRotMatrix
   case (2)
           SolidState=.true.
           OMflag=.true.
           OMweight = rparam('OMweight')
           OMtol = rparam('OMtol')
           call putlin (2,'Crystal mode with origin '//
*                  'forced alignment with internal metal')
           call putlin (2,'Do not forget to upload a matrix '//
*                  'by a .omr file')
           call initRotMatrix

   case default
       CALL ERRMSG('wrong crystal mode! select 0 or 1')
   end select
   if (cryNDTENSO.ne.1.and.cryntenso.ne.1) then
       write(6,*) 'OPTION NOT YET IMPLEMENTED'
       stop
   end if
   if (cryNDTENSO*cryntenso.gt.maxtenscry/2) then
     CALL ERRMSG('Too many tensors!')
     stop
   endif
   if (.not.option('append')) ndipcry=0
   n=ndipcry
   call getcrydip(1,mode)
   close(1)
   if (haverr()) go to 900
   call putlin (2,'Pseudo contact shifts constraint '//
*               'file '//strq(filnam)//
*               ' read, '//plural(ndipcry-n,'constraint')//'.')
```


WinMerge - [readf.f - readf.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\readf.f

```
           CALL ERRMSG('Too many tensors!')
           stop
         endif
         if (.not.option('append')) ndip=0
         n=ndip
         call getdip(1,mode)
         close(1)
         if (haverr()) go to 900
         call putlin (2,'Pseudo contact shifts constraint '
     *                 'file '//strq(filnam)//
     *                 ' read, '//plural(ndip-n,'constraint'
```

Ln: 366 Col: 72/72 Car: 72/72 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\readf.f

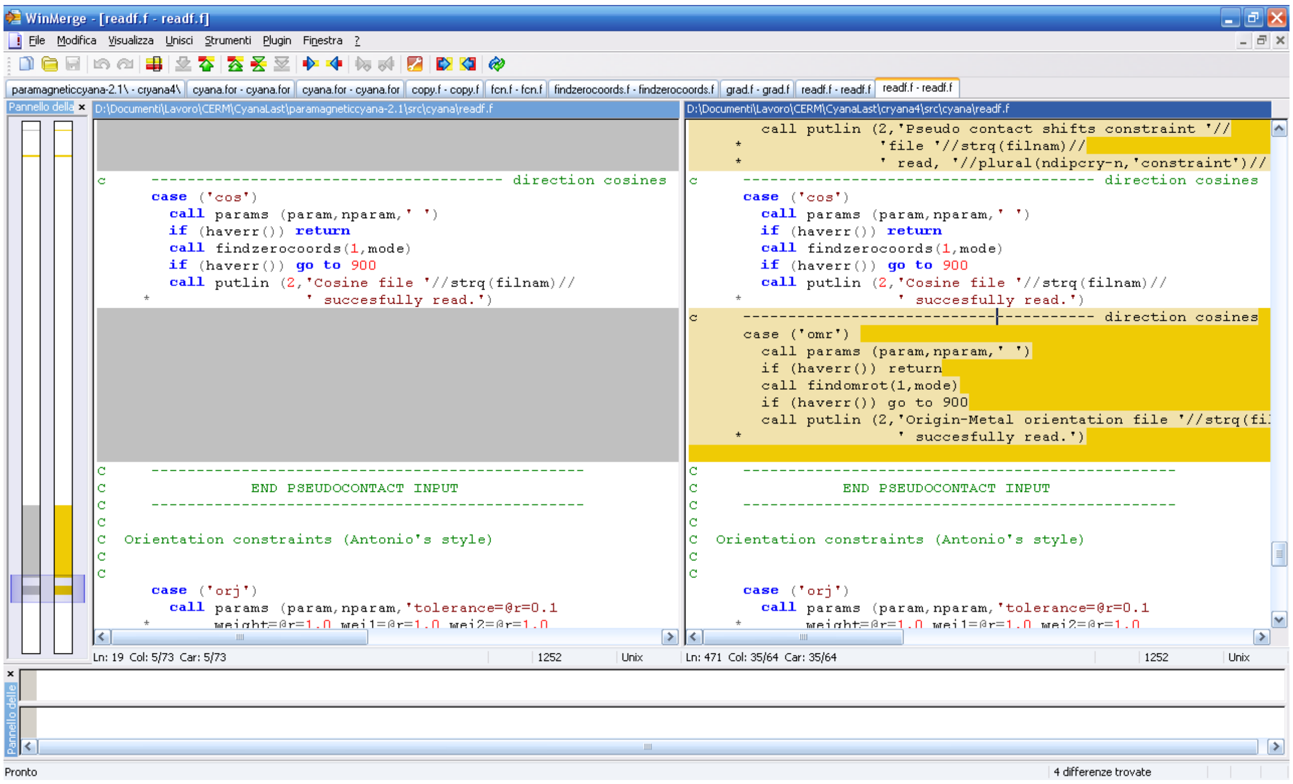
```
           CALL ERRMSG('Too many tensors!')
           stop
         endif
         if (.not.option('append')) ndip=0
         n=ndip
         call getdip(1,mode)
         close(1)
         if (haverr()) go to 900
         call putlin (2,'Pseudo contact shifts constraint '
     *                 'file '//strq(filnam)//
     *                 ' read, '//plural(ndip-n,'constraint'
c      ---------------------------------------------- pse
       case ('cry')
         call params (param,nparam,'tolerance=@r=0.4 crysta
     *       'weight=@r=1.0 tensors=@i=1 perc=@r=0.1 dtens=
     *       'OMweight=@r=10.0 OMtol=@r=0.1 '//
     *       'symmetry=none|P21212|P212121|P222|P2221|=none
!     *        'P=@r=4. T=@r=4. O=@r=4. append')
         if (haverr()) return
         OMflag=.false.
         crytoldip=rparam('tolerance')
         cryncrystal=iparam('crystal')
         crywdip=rparam('weight')
         cryntenso=iparam('tensors')
         crypseperc=rparam('perc')
         cryNDTENSO=iparam('dtens')
         call getpar ('symmetry',symmetry) ! da eliminare i
         crystalmode=cryncrystal
```

Ln: 390 Col: 7/70 Car: 7/70 EOL: LF 1252 Mescolato

```
         if (haverr()) return

         if (haverr()) return
```

Pronto 4 differenze trovate

4) add omr case


WinMerge - [readf.f - readf.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\readf.f

```
c      ---------------------------------------- direction cosines
       case ('cos')
         call params (param,nparam,' ')
         if (haverr()) return
         call findzerocoords(1,mode)
         if (haverr()) go to 900
         call putlin (2,'Cosine file '//strq(filnam)//
     *                 ' succesfully read.')
C      --------------------------------------------------
C                END PSEUDOCONTACT INPUT
C      --------------------------------------------------
C
C   Orientation constraints (Antonio's style)
C
C
       case ('orj')
         call params (param,nparam,'tolerance=@r=0.1
     *        weight=@r=1.0 wei1=@r=1.0 wei2=@r=1.0
```

Ln: 19 Col: 5/73 Car: 5/73 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\readf.f

```
         call putlin (2,'Pseudo contact shifts constraint '//
     *                 'file '//strq(filnam)//
     *                 ' read, '//plural(ndipcry-n,'constraint')//
c      ---------------------------------------- direction cosines
       case ('cos')
         call params (param,nparam,' ')
         if (haverr()) return
         call findzerocoords(1,mode)
         if (haverr()) go to 900
         call putlin (2,'Cosine file '//strq(filnam)//
     *                 ' succesfully read.')
c      ---------------------------------------- direction cosines
       case ('omr')
         call params (param,nparam,' ')
         if (haverr()) return
         call findomrot(1,mode)
         if (haverr()) go to 900
         call putlin (2,'Origin-Metal orientation file '//strq(fi
     *                 ' succesfully read.')

C      --------------------------------------------------
C                END PSEUDOCONTACT INPUT
C      --------------------------------------------------
C
C   Orientation constraints (Antonio's style)
C
C
       case ('orj')
         call params (param,nparam,'tolerance=@r=0.1
     *        weight=@r=1.0 wei1=@r=1.0 wei2=@r=1.0
```

Ln: 471 Col: 35/64 Car: 35/64 1252 Unix

Pronto 4 differenze trovate

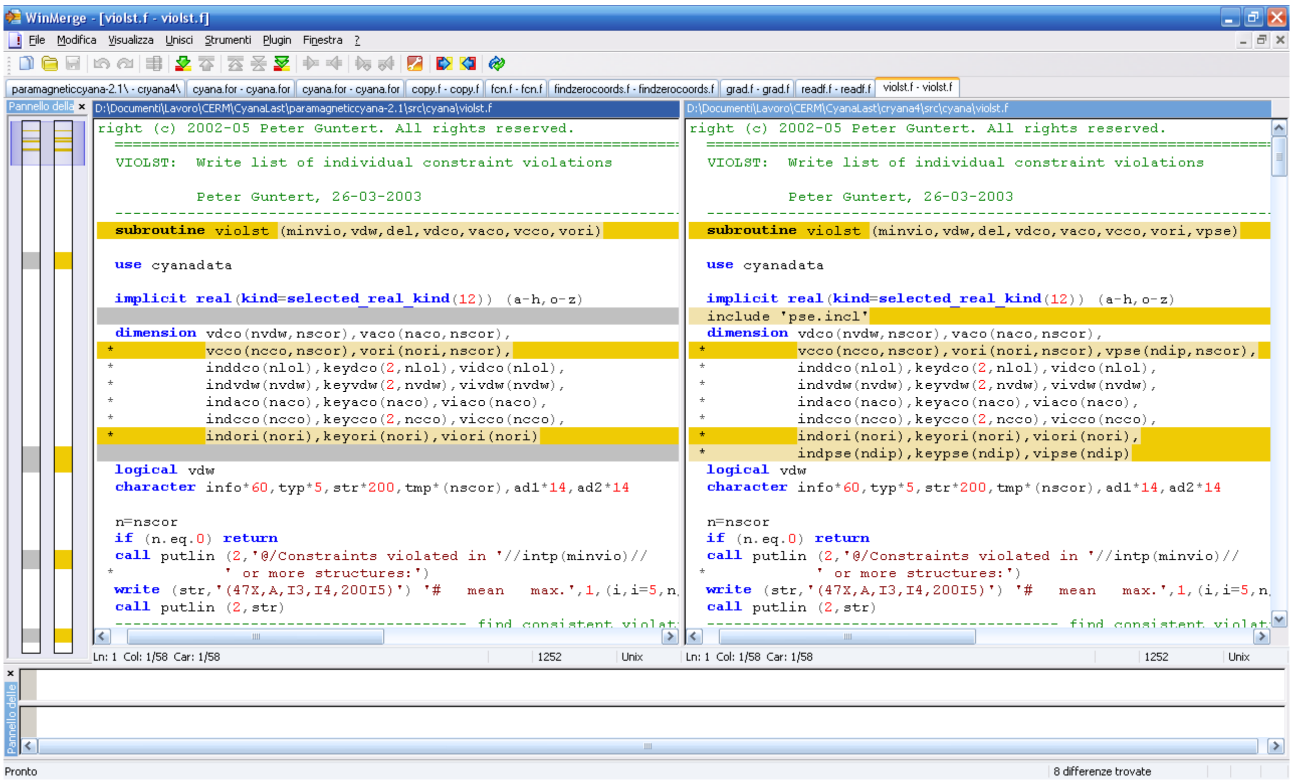
violst.f

1) add

```
    include  'pse.incl'
```

2) add variables

```
     vpse(ndip,nscor),indpse(ndip),keypse(ndip),vipse(ndip)
```



WinMerge - [violst.f - violst.f]

paramagneticcyana-2.1\ - cryana4\ | cyana.for - cyana.for | cyana.for - cyana.for | copy.f - copy.f | fcn.f - fcn.f | findzerocoords.f - findzerocoords.f | grad.f - grad.f | readf.f - readf.f | violst.f - violst.f

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\violst.f

```
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  ====================================================================
  VIOLST:  Write list of individual constraint violations

           Peter Guntert, 26-03-2003
  --------------------------------------------------------------------
  subroutine violst (minvio,vdw,del,vdco,vaco,vcco,vori)

  use cyanadata

  implicit real(kind=selected_real_kind(12)) (a-h,o-z)

  dimension vdco(nvdw,nscor),vaco(naco,nscor),
 *          vcco(ncco,nscor),vori(nori,nscor),
 *          inddco(nlol),keydco(2,nlol),vidco(nlol),
 *          indvdw(nvdw),keyvdw(2,nvdw),vivdw(nvdw),
 *          indaco(naco),keyaco(naco),viaco(naco),
 *          indcco(ncco),keycco(2,ncco),vicco(ncco),
 *          indori(nori),keyori(nori),viori(nori)

  logical vdw
  character info*60,typ*5,str*200,tmp*(nscor),ad1*14,ad2*14

  n=nscor
  if (n.eq.0) return
  call putlin (2,'@/Constraints violated in '//intp(minvio)//
 *     ' or more structures:')
  write (str,'(47X,A,I3,I4,200I5)') '#   mean   max.',1,(i,i=5,n,
  call putlin (2,str)
  ---------------------------------------- find consistent violat
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\violst.f

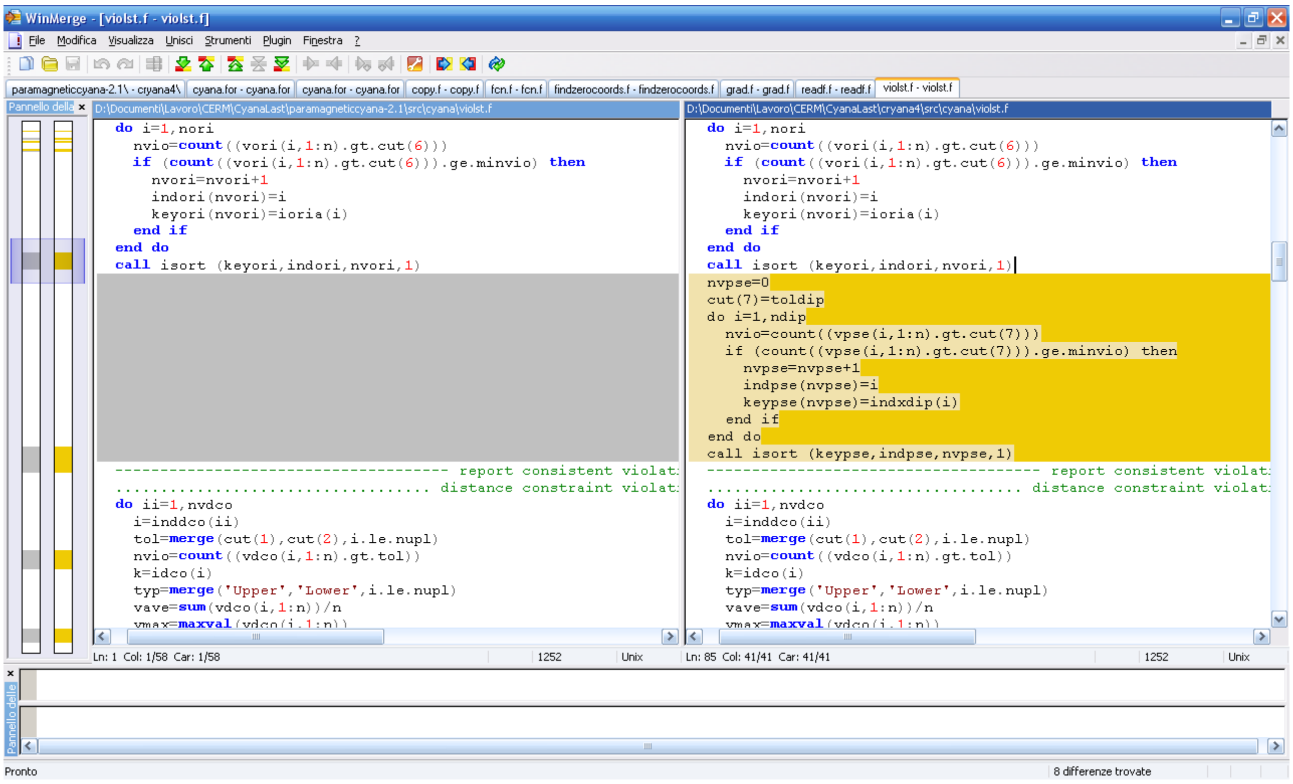
```
right (c) 2002-05 Peter Guntert. All rights reserved.
  ====================================================================
  VIOLST:  Write list of individual constraint violations

           Peter Guntert, 26-03-2003
  --------------------------------------------------------------------
  subroutine violst (minvio,vdw,del,vdco,vaco,vcco,vori,vpse)

  use cyanadata

  implicit real(kind=selected_real_kind(12)) (a-h,o-z)
  include 'pse.incl'
  dimension vdco(nvdw,nscor),vaco(naco,nscor),
 *          vcco(ncco,nscor),vori(nori,nscor),vpse(ndip,nscor),
 *          inddco(nlol),keydco(2,nlol),vidco(nlol),
 *          indvdw(nvdw),keyvdw(2,nvdw),vivdw(nvdw),
 *          indaco(naco),keyaco(naco),viaco(naco),
 *          indcco(ncco),keycco(2,ncco),vicco(ncco),
 *          indori(nori),keyori(nori),viori(nori),
 *          indpse(ndip),keypse(ndip),vipse(ndip)
  logical vdw
  character info*60,typ*5,str*200,tmp*(nscor),ad1*14,ad2*14

  n=nscor
  if (n.eq.0) return
  call putlin (2,'@/Constraints violated in '//intp(minvio)//
 *     ' or more structures:')
  write (str,'(47X,A,I3,I4,200I5)') '#   mean   max.',1,(i,i=5,n,
  call putlin (2,str)
  ---------------------------------------- find consistent violat
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

Pronto   8 differenze trovate

3) add

```
    nvpse=0
    cut(7)=toldip
    do i=1,ndip
      nvio=count((vpse(i,1:n).gt.cut(7)))
      if (count((vpse(i,1:n).gt.cut(7))).ge.minvio) then
        nvpse=nvpse+1
        indpse(nvpse)=i
        keypse(nvpse)=indxdip(i)
      end if
    end do
    call isort (keypse,indpse,nvpse,1)
```


WinMerge - [violst.f - violst.f]
File Modifica Visualizza Unisci Strumenti Plugin Finestra ?
paramagneticcyana-2.1\ - cryana4\ | cyana.for - cyana.for | cyana.for - cyana.for | copy.f - copy.f | fcn.f - fcn.f | findzerocoords.f - findzerocoords.f | grad.f - grad.f | readf.f - readf.f | violst.f - violst.f
Pannello della
Pannello delle
Ln: 1 Col: 1/58 Car: 1/58 1252 Unix
Ln: 85 Col: 41/41 Car: 41/41 1252 Unix
Pronto
8 differenze trovate

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\violst.f

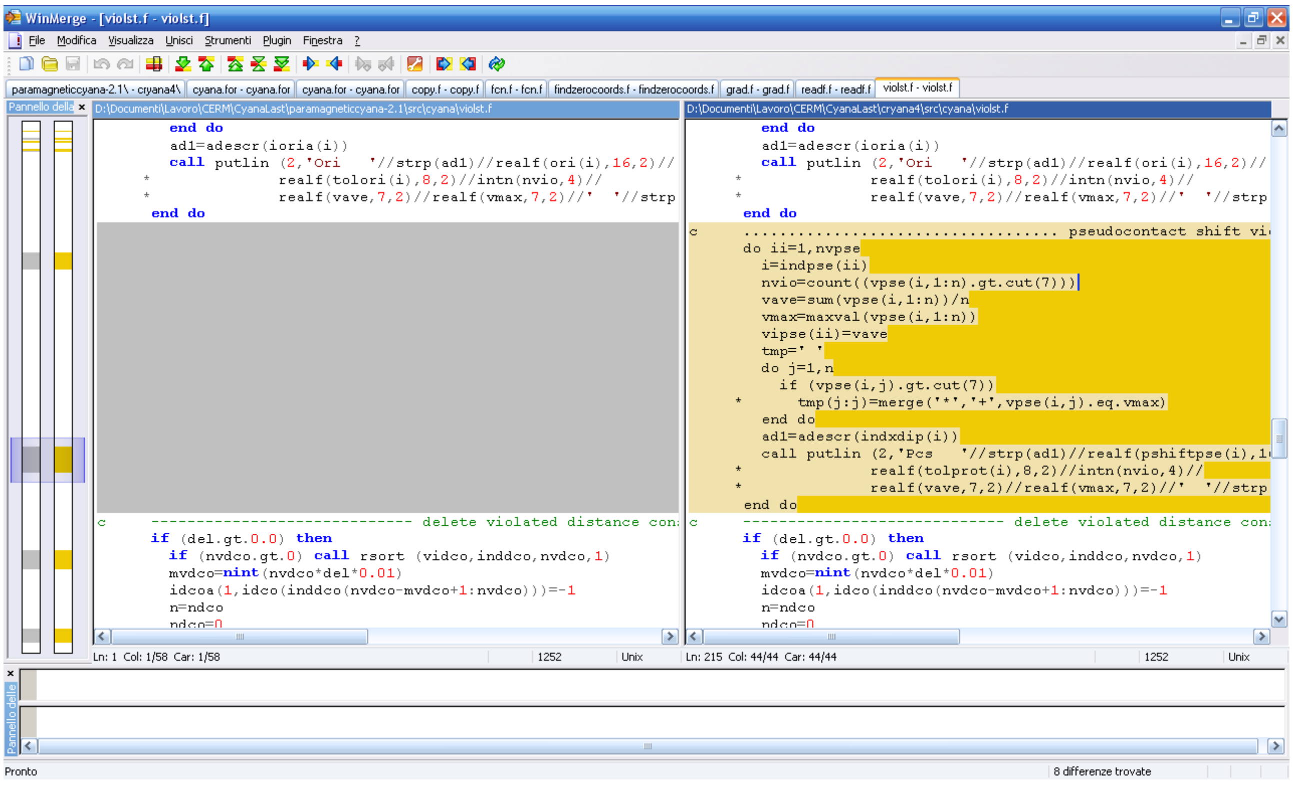
```
  do i=1,nori
    nvio=count((vori(i,1:n).gt.cut(6)))
    if (count((vori(i,1:n).gt.cut(6))).ge.minvio) then
      nvori=nvori+1
      indori(nvori)=i
      keyori(nvori)=ioria(i)
    end if
  end do
  call isort (keyori,indori,nvori,1)









  ----------------------------------- report consistent violat
  ................................. distance constraint violat
  do ii=1,nvdco
    i=inddco(ii)
    tol=merge(cut(1),cut(2),i.le.nupl)
    nvio=count((vdco(i,1:n).gt.tol))
    k=idco(i)
    typ=merge('Upper','Lower',i.le.nupl)
    vave=sum(vdco(i,1:n))/n
    vmax=maxval(vdco(i,1:n))
```

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\violst.f

```
  do i=1,nori
    nvio=count((vori(i,1:n).gt.cut(6)))
    if (count((vori(i,1:n).gt.cut(6))).ge.minvio) then
      nvori=nvori+1
      indori(nvori)=i
      keyori(nvori)=ioria(i)
    end if
  end do
  call isort (keyori,indori,nvori,1)
  nvpse=0
  cut(7)=toldip
  do i=1,ndip
    nvio=count((vpse(i,1:n).gt.cut(7)))
    if (count((vpse(i,1:n).gt.cut(7))).ge.minvio) then
      nvpse=nvpse+1
      indpse(nvpse)=i
      keypse(nvpse)=indxdip(i)
    end if
  end do
  call isort (keypse,indpse,nvpse,1)
  ----------------------------------- report consistent violat
  ................................. distance constraint violat
  do ii=1,nvdco
    i=inddco(ii)
    tol=merge(cut(1),cut(2),i.le.nupl)
    nvio=count((vdco(i,1:n).gt.tol))
    k=idco(i)
    typ=merge('Upper','Lower',i.le.nupl)
    vave=sum(vdco(i,1:n))/n
    vmax=maxval(vdco(i,1:n))
```

4) add

```
c      .................................. pseudocontact shift violations
       do ii=1,nvpse
         i=indpse(ii)
         nvio=count((vpse(i,1:n).gt.cut(7)))
         vave=sum(vpse(i,1:n))/n
         vmax=maxval(vpse(i,1:n))
         vipse(ii)=vave
         tmp=' '
         do j=1,n
           if (vpse(i,j).gt.cut(7))
     *       tmp(j:j)=merge('*','+',vpse(i,j).eq.vmax)
         end do
         ad1=adescr(indxdip(i))
         call putlin (2,'Pcs    '//strp(ad1)//realf(pshiftpse(i),16,2)//
     *              realf(tolprot(i),8,2)//intn(nvio,4)//
     *              realf(vave,7,2)//realf(vmax,7,2)//'  '//strp(tmp))
       end do
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\violst.f

```
          end do
          ad1=adescr(ioria(i))
          call putlin (2,'Ori   '//strp(ad1)//realf(ori(i),16,2)//
     *                realf(tolori(i),8,2)//intn(nvio,4)//
     *                realf(vave,7,2)//realf(vmax,7,2)//'  '//strp
        end do
c       ----------------------------- delete violated distance con
        if (del.gt.0.0) then
          if (nvdco.gt.0) call rsort (vidco,inddco,nvdco,1)
          mvdco=nint(nvdco*del*0.01)
          idcoa(1,idco(inddco(nvdco-mvdco+1:nvdco)))=-1
          n=ndco
          ndco=0
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

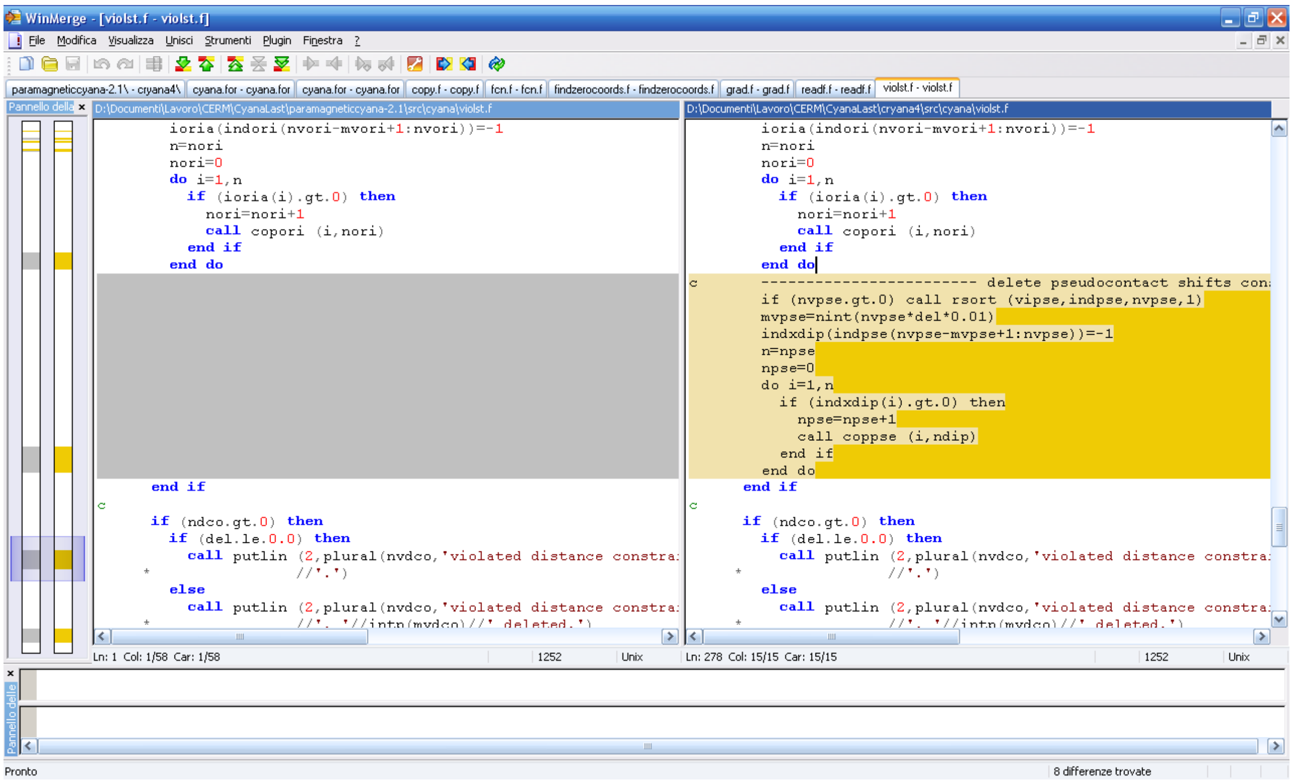
D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\violst.f

```
          end do
          ad1=adescr(ioria(i))
          call putlin (2,'Ori   '//strp(ad1)//realf(ori(i),16,2)//
     *                realf(tolori(i),8,2)//intn(nvio,4)//
     *                realf(vave,7,2)//realf(vmax,7,2)//'  '//strp
        end do
c       .................................. pseudocontact shift vi
        do ii=1,nvpse
          i=indpse(ii)
          nvio=count((vpse(i,1:n).gt.cut(7)))
          vave=sum(vpse(i,1:n))/n
          vmax=maxval(vpse(i,1:n))
          vipse(ii)=vave
          tmp=' '
          do j=1,n
            if (vpse(i,j).gt.cut(7))
     *        tmp(j:j)=merge('*','+',vpse(i,j).eq.vmax)
          end do
          ad1=adescr(indxdip(i))
          call putlin (2,'Pcs   '//strp(ad1)//realf(pshiftpse(i),1
     *                realf(tolprot(i),8,2)//intn(nvio,4)//
     *                realf(vave,7,2)//realf(vmax,7,2)//'  '//strp
        end do
c       ----------------------------- delete violated distance con
        if (del.gt.0.0) then
          if (nvdco.gt.0) call rsort (vidco,inddco,nvdco,1)
          mvdco=nint(nvdco*del*0.01)
          idcoa(1,idco(inddco(nvdco-mvdco+1:nvdco)))=-1
          n=ndco
          ndco=0
```

Ln: 215 Col: 44/44 Car: 44/44   1252   Unix

5) add

```
c       ------------------------ delete pseudocontact shifts constraints
        if (nvpse.gt.0) call rsort (vipse,indpse,nvpse,1)
        mvpse=nint(nvpse*del*0.01)
        indxdip(indpse(nvpse-mvpse+1:nvpse))=-1
        n=npse
        npse=0
        do i=1,n
          if (indxdip(i).gt.0) then
            npse=npse+1
            call coppse (i,ndip)
          end if
        end do
```



WinMerge - [violst.f - violst.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\violst.f

```
         ioria(indori(nvori-mvori+1:nvori))=-1
         n=nori
         nori=0
         do i=1,n
           if (ioria(i).gt.0) then
             nori=nori+1
             call copori (i,nori)
           end if
         end do
       end if
c
       if (ndco.gt.0) then
         if (del.le.0.0) then
           call putlin (2,plural(nvdco,'violated distance constra
     *                 //'.')
         else
           call putlin (2,plural(nvdco,'violated distance constra
     *                 //', '//intp(mvdco)//' deleted.')
```

Ln: 1 Col: 1/58 Car: 1/58   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\violst.f

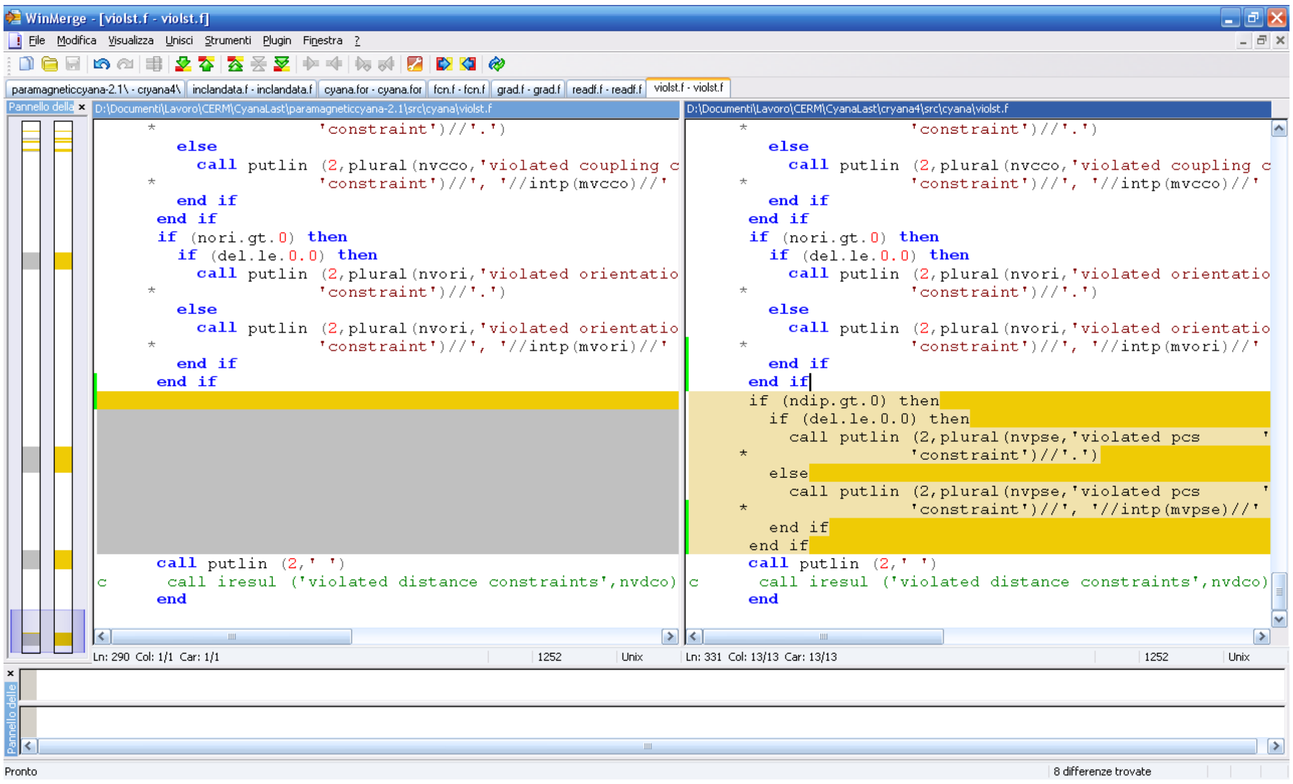
```
         ioria(indori(nvori-mvori+1:nvori))=-1
         n=nori
         nori=0
         do i=1,n
           if (ioria(i).gt.0) then
             nori=nori+1
             call copori (i,nori)
           end if
         end do
c        ---------------------- delete pseudocontact shifts con
         if (nvpse.gt.0) call rsort (vipse,indpse,nvpse,1)
         mvpse=nint(nvpse*del*0.01)
         indxdip(indpse(nvpse-mvpse+1:nvpse))=-1
         n=npse
         npse=0
         do i=1,n
           if (indxdip(i).gt.0) then
             npse=npse+1
             call coppse (i,ndip)
           end if
         end do
       end if
c
       if (ndco.gt.0) then
         if (del.le.0.0) then
           call putlin (2,plural(nvdco,'violated distance constra
     *                 //'.')
         else
           call putlin (2,plural(nvdco,'violated distance constra
     *                 //', '//intp(mvdco)//' deleted.')
```

Ln: 278 Col: 15/15 Car: 15/15   1252   Unix

Pronto   8 differenze trovate

6) add

```
   if (ndip.gt.0) then
     if (del.le.0.0) then
       call putlin (2,plural(nvpse,'violated pcs       '//
 *                 'constraint')//'.')
     else
       call putlin (2,plural(nvpse,'violated pcs       '//
 *                 'constraint')//', '//intp(mvpse)//' deleted.')
     end if
   end if
```



WinMerge - [violst.f - violst.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\violst.f

```
     *                 'constraint')//'.')
         else
           call putlin (2,plural(nvcco,'violated coupling c
     *                 'constraint')//', '//intp(mvcco)//'
         end if
       end if
       if (nori.gt.0) then
         if (del.le.0.0) then
           call putlin (2,plural(nvori,'violated orientatio
     *                 'constraint')//'.')
         else
           call putlin (2,plural(nvori,'violated orientatio
     *                 'constraint')//', '//intp(mvori)//'
         end if
       end if
       call putlin (2,' ')
c       call iresul ('violated distance constraints',nvdco)
       end
```

Ln: 290 Col: 1/1 Car: 1/1   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\violst.f

```
     *                 'constraint')//'.')
         else
           call putlin (2,plural(nvcco,'violated coupling c
     *                 'constraint')//', '//intp(mvcco)//'
         end if
       end if
       if (nori.gt.0) then
         if (del.le.0.0) then
           call putlin (2,plural(nvori,'violated orientatio
     *                 'constraint')//'.')
         else
           call putlin (2,plural(nvori,'violated orientatio
     *                 'constraint')//', '//intp(mvori)//'
         end if
       end if
       if (ndip.gt.0) then
         if (del.le.0.0) then
           call putlin (2,plural(nvpse,'violated pcs       '
     *                 'constraint')//'.')
         else
           call putlin (2,plural(nvpse,'violated pcs       '
     *                 'constraint')//', '//intp(mvpse)//'
         end if
       end if
       call putlin (2,' ')
c       call iresul ('violated distance constraints',nvdco)
       end
```

Ln: 331 Col: 13/13 Car: 13/13   1252   Unix

Pronto   8 differenze trovate

viosta.f

1) add

```
include  'pse.incl'
```

2) add variables

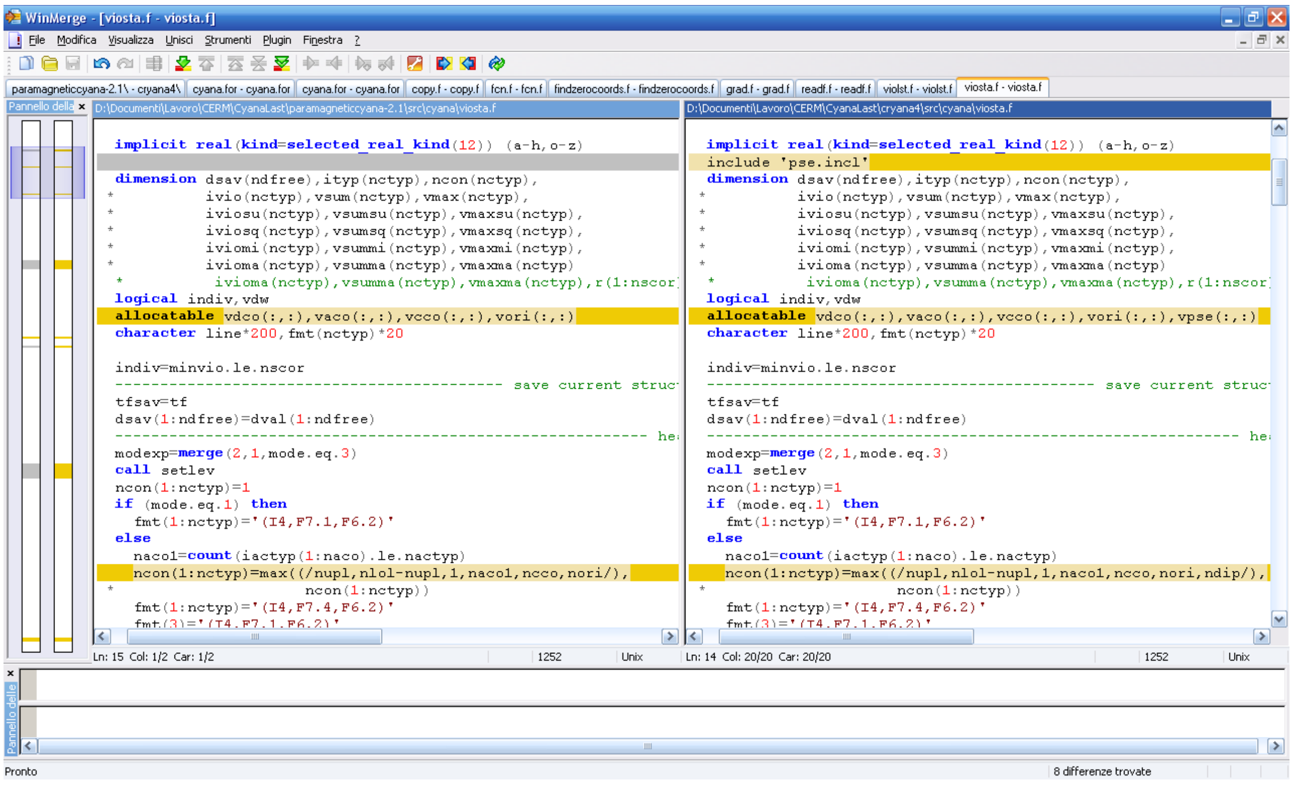
```
 vpse(:,:),
```

3) change

```
ncon(1:nctyp)=max((/nupl,nlol-nupl,1,naco1,ncco,nori/),
```

→

```
ncon(1:nctyp)=max((/nupl,nlol-nupl,1,naco1,ncco,nori,ndip/),
```



WinMerge - [viosta.f - viosta.f]

paramagneticcyana-2.1\ - cryana4\ | cyana.for - cyana.for | cyana.for - cyana.for | copy.f - copy.f | fcn.f - fcn.f | findzerocoords.f - findzerocoords.f | grad.f - grad.f | readf.f - readf.f | violst.f - violst.f | viosta.f - viosta.f

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\viosta.f

```
  implicit real(kind=selected_real_kind(12))  (a-h,o-z)

  dimension dsav(ndfree),ityp(nctyp),ncon(nctyp),
 *          ivio(nctyp),vsum(nctyp),vmax(nctyp),
 *          iviosu(nctyp),vsumsu(nctyp),vmaxsu(nctyp),
 *          iviosq(nctyp),vsumsq(nctyp),vmaxsq(nctyp),
 *          iviomi(nctyp),vsummi(nctyp),vmaxmi(nctyp),
 *          ivioma(nctyp),vsumma(nctyp),vmaxma(nctyp)
  *          ivioma(nctyp),vsumma(nctyp),vmaxma(nctyp),r(1:nscor
  logical indiv,vdw
  allocatable vdco(:,:),vaco(:,:),vcco(:,:),vori(:,:)
  character line*200,fmt(nctyp)*20

  indiv=minvio.le.nscor
  ------------------------------------------- save current struc
  tfsav=tf
  dsav(1:ndfree)=dval(1:ndfree)
  ------------------------------------------------------------ he
  modexp=merge(2,1,mode.eq.3)
  call setlev
  ncon(1:nctyp)=1
  if (mode.eq.1) then
    fmt(1:nctyp)='(I4,F7.1,F6.2)'
  else
    naco1=count(iactyp(1:naco).le.nactyp)
    ncon(1:nctyp)=max((/nupl,nlol-nupl,1,naco1,ncco,nori/),
 *                       ncon(1:nctyp))
    fmt(1:nctyp)='(I4,F7.4,F6.2)'
    fmt(3)='(I4,F7.1,F6.2)'
```

Ln: 15 Col: 1/2 Car: 1/2   1252   Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\viosta.f

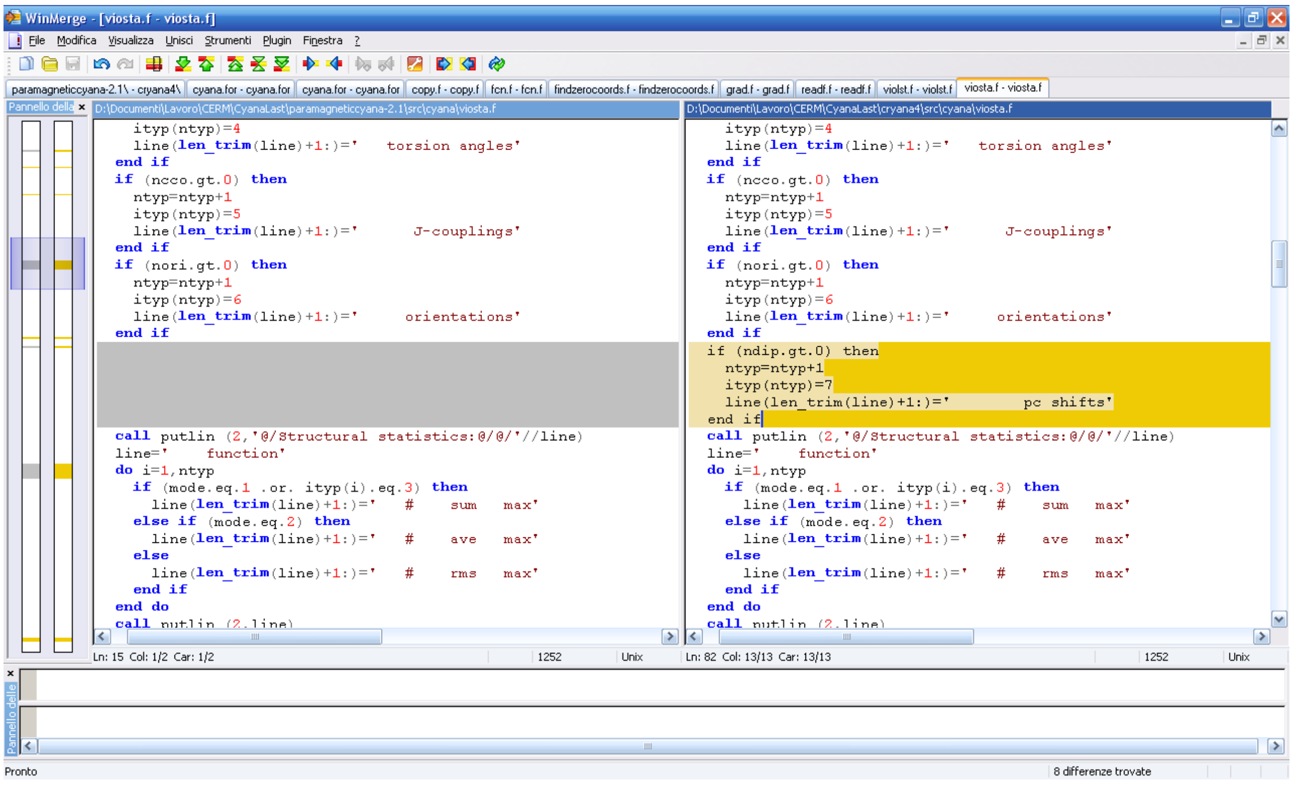
```
  implicit real(kind=selected_real_kind(12))  (a-h,o-z)
  include 'pse.incl'
  dimension dsav(ndfree),ityp(nctyp),ncon(nctyp),
 *          ivio(nctyp),vsum(nctyp),vmax(nctyp),
 *          iviosu(nctyp),vsumsu(nctyp),vmaxsu(nctyp),
 *          iviosq(nctyp),vsumsq(nctyp),vmaxsq(nctyp),
 *          iviomi(nctyp),vsummi(nctyp),vmaxmi(nctyp),
 *          ivioma(nctyp),vsumma(nctyp),vmaxma(nctyp)
  *          ivioma(nctyp),vsumma(nctyp),vmaxma(nctyp),r(1:nscor
  logical indiv,vdw
  allocatable vdco(:,:),vaco(:,:),vcco(:,:),vori(:,:),vpse(:,:)
  character line*200,fmt(nctyp)*20

  indiv=minvio.le.nscor
  ------------------------------------------- save current struc
  tfsav=tf
  dsav(1:ndfree)=dval(1:ndfree)
  ------------------------------------------------------------ he
  modexp=merge(2,1,mode.eq.3)
  call setlev
  ncon(1:nctyp)=1
  if (mode.eq.1) then
    fmt(1:nctyp)='(I4,F7.1,F6.2)'
  else
    naco1=count(iactyp(1:naco).le.nactyp)
    ncon(1:nctyp)=max((/nupl,nlol-nupl,1,naco1,ncco,nori,ndip/),
 *                       ncon(1:nctyp))
    fmt(1:nctyp)='(I4,F7.4,F6.2)'
    fmt(3)='(I4,F7.1,F6.2)'
```

Ln: 14 Col: 20/20 Car: 20/20   1252   Unix

Pronto   8 differenze trovate

4) add

```
if (ndip.gt.0) then
  ntyp=ntyp+1
  ityp(ntyp)=7
  line(len_trim(line)+1:)='         pc shifts'
end if
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\viosta.f

```
      ityp(ntyp)=4
      line(len_trim(line)+1:)='   torsion angles'
   end if
   if (ncco.gt.0) then
      ntyp=ntyp+1
      ityp(ntyp)=5
      line(len_trim(line)+1:)='      J-couplings'
   end if
   if (nori.gt.0) then
      ntyp=ntyp+1
      ityp(ntyp)=6
      line(len_trim(line)+1:)='     orientations'
   end if




   call putlin (2,'@/Structural statistics:@/@/'//line)
   line='     function'
   do i=1,ntyp
      if (mode.eq.1 .or. ityp(i).eq.3) then
         line(len_trim(line)+1:)='   #     sum    max'
      else if (mode.eq.2) then
         line(len_trim(line)+1:)='   #     ave    max'
      else
         line(len_trim(line)+1:)='   #     rms    max'
      end if
   end do
   call putlin (2,line)
```

Ln: 15 Col: 1/2 Car: 1/2 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\viosta.f

```
      ityp(ntyp)=4
      line(len_trim(line)+1:)='   torsion angles'
   end if
   if (ncco.gt.0) then
      ntyp=ntyp+1
      ityp(ntyp)=5
      line(len_trim(line)+1:)='      J-couplings'
   end if
   if (nori.gt.0) then
      ntyp=ntyp+1
      ityp(ntyp)=6
      line(len_trim(line)+1:)='     orientations'
   end if
   if (ndip.gt.0) then
      ntyp=ntyp+1
      ityp(ntyp)=7
      line(len_trim(line)+1:)='        pc shifts'
   end if
   call putlin (2,'@/Structural statistics:@/@/'//line)
   line='     function'
   do i=1,ntyp
      if (mode.eq.1 .or. ityp(i).eq.3) then
         line(len_trim(line)+1:)='   #     sum    max'
      else if (mode.eq.2) then
         line(len_trim(line)+1:)='   #     ave    max'
      else
         line(len_trim(line)+1:)='   #     rms    max'
      end if
   end do
   call putlin (2,line)
```

Ln: 82 Col: 13/13 Car: 13/13 1252 Unix

5) change

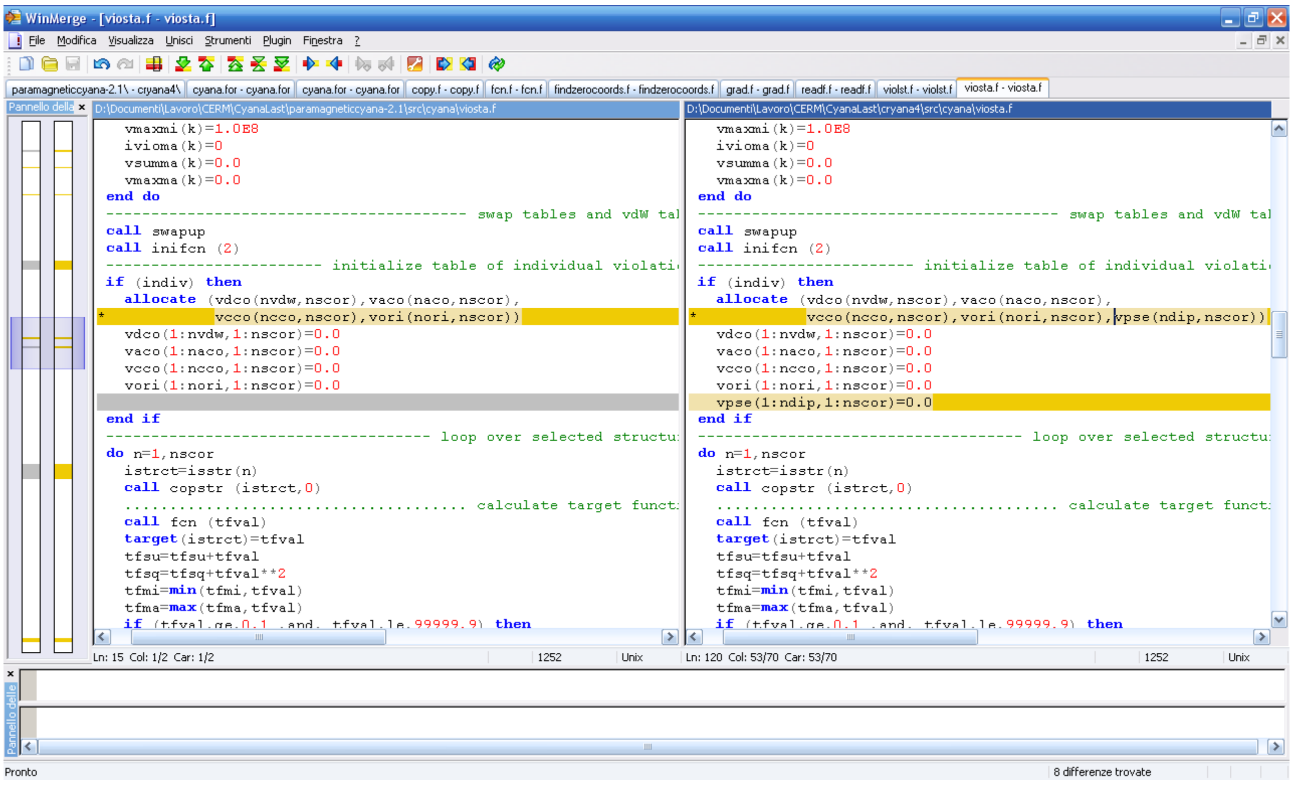
```
   allocate (vdco(nvdw,nscor),vaco(naco,nscor),
*           vcco(ncco,nscor),vori(nori,nscor))
```

→

```
   allocate (vdco(nvdw,nscor),vaco(naco,nscor),
*           vcco(ncco,nscor),vori(nori,nscor),vpse(ndip,nscor))
```

6) add

```
vpse(1:ndip,1:nscor)=0.0
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\viosta.f

```
     vmaxmi(k)=1.0E8
     ivioma(k)=0
     vsumma(k)=0.0
     vmaxma(k)=0.0
  end do
c ---------------------------------------- swap tables and vdW tal
  call swapup
  call inifcn (2)
c ------------------------ initialize table of individual violati
  if (indiv) then
     allocate (vdco(nvdw,nscor),vaco(naco,nscor),
*             vcco(ncco,nscor),vori(nori,nscor))
     vdco(1:nvdw,1:nscor)=0.0
     vaco(1:naco,1:nscor)=0.0
     vcco(1:ncco,1:nscor)=0.0
     vori(1:nori,1:nscor)=0.0

  end if
c ------------------------------------ loop over selected structu
  do n=1,nscor
     istrct=isstr(n)
     call copstr (istrct,0)
c .................................... calculate target funct
     call fcn (tfval)
     target(istrct)=tfval
     tfsu=tfsu+tfval
     tfsq=tfsq+tfval**2
     tfmi=min(tfmi,tfval)
     tfma=max(tfma,tfval)
     if (tfval.ge.0.1 .and. tfval.le.99999.9) then
```

Ln: 15 Col: 1/2 Car: 1/2 1252 Unix

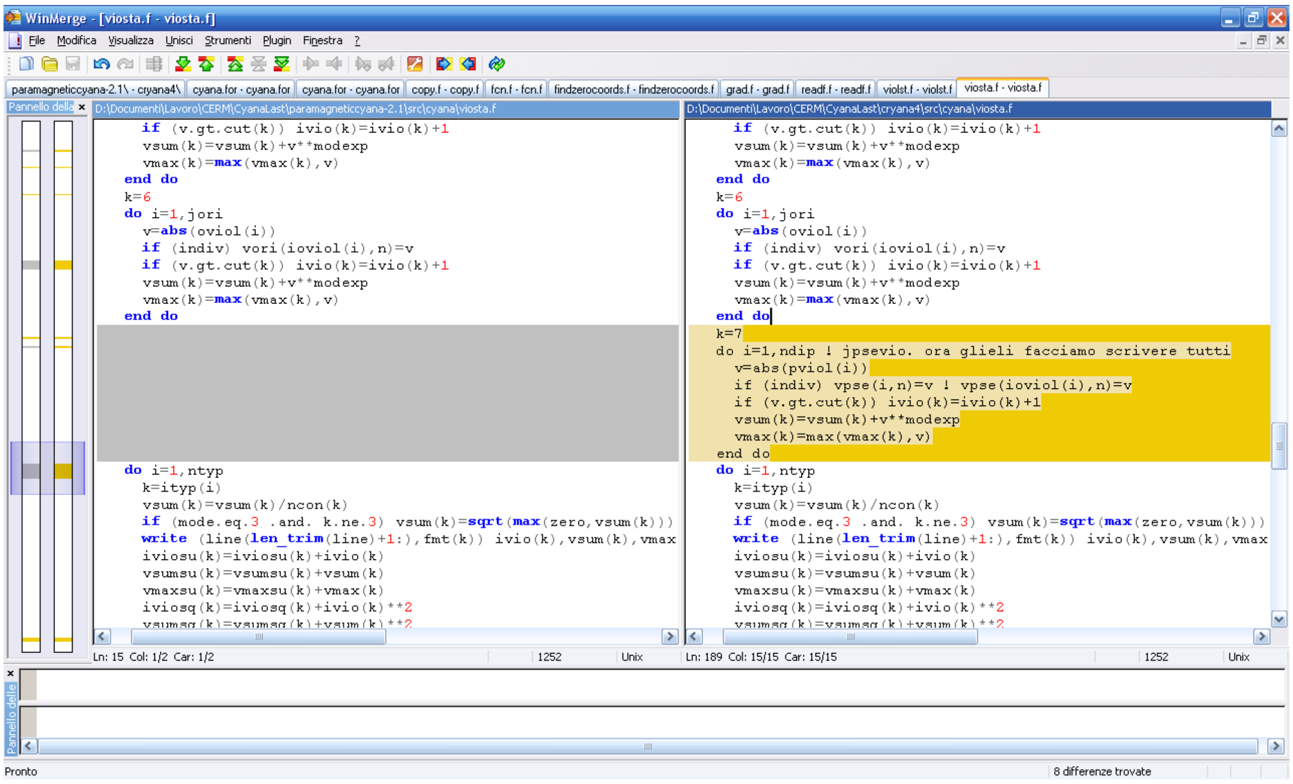
D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\viosta.f

```
     vmaxmi(k)=1.0E8
     ivioma(k)=0
     vsumma(k)=0.0
     vmaxma(k)=0.0
  end do
c ---------------------------------------- swap tables and vdW tal
  call swapup
  call inifcn (2)
c ------------------------ initialize table of individual violati
  if (indiv) then
     allocate (vdco(nvdw,nscor),vaco(naco,nscor),
*             vcco(ncco,nscor),vori(nori,nscor),vpse(ndip,nscor))
     vdco(1:nvdw,1:nscor)=0.0
     vaco(1:naco,1:nscor)=0.0
     vcco(1:ncco,1:nscor)=0.0
     vori(1:nori,1:nscor)=0.0
     vpse(1:ndip,1:nscor)=0.0
  end if
c ------------------------------------ loop over selected structu
  do n=1,nscor
     istrct=isstr(n)
     call copstr (istrct,0)
c .................................... calculate target funct
     call fcn (tfval)
     target(istrct)=tfval
     tfsu=tfsu+tfval
     tfsq=tfsq+tfval**2
     tfmi=min(tfmi,tfval)
     tfma=max(tfma,tfval)
     if (tfval.ge.0.1 .and. tfval.le.99999.9) then
```

Ln: 120 Col: 53/70 Car: 53/70 1252 Unix

7) add

```
k=7
do i=1,ndip ! jpsevio. ora glieli facciamo scrivere tutti
  v=abs(pviol(i))
  if (indiv) vpse(i,n)=v ! vpse(ioviol(i),n)=v
  if (v.gt.cut(k)) ivio(k)=ivio(k)+1
  vsum(k)=vsum(k)+v**modexp
  vmax(k)=max(vmax(k),v)
end do
```



D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\viosta.f

```
      if (v.gt.cut(k)) ivio(k)=ivio(k)+1
      vsum(k)=vsum(k)+v**modexp
      vmax(k)=max(vmax(k),v)
    end do
    k=6
    do i=1,jori
      v=abs(oviol(i))
      if (indiv) vori(ioviol(i),n)=v
      if (v.gt.cut(k)) ivio(k)=ivio(k)+1
      vsum(k)=vsum(k)+v**modexp
      vmax(k)=max(vmax(k),v)
    end do







    do i=1,ntyp
      k=ityp(i)
      vsum(k)=vsum(k)/ncon(k)
      if (mode.eq.3 .and. k.ne.3) vsum(k)=sqrt(max(zero,vsum(k)))
      write (line(len_trim(line)+1:),fmt(k)) ivio(k),vsum(k),vmax
      iviosu(k)=iviosu(k)+ivio(k)
      vsumsu(k)=vsumsu(k)+vsum(k)
      vmaxsu(k)=vmaxsu(k)+vmax(k)
      iviosq(k)=iviosq(k)+ivio(k)**2
      vsumsq(k)=vsumsq(k)+vsum(k)**2
```

Ln: 15 Col: 1/2 Car: 1/2 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\viosta.f

```
      if (v.gt.cut(k)) ivio(k)=ivio(k)+1
      vsum(k)=vsum(k)+v**modexp
      vmax(k)=max(vmax(k),v)
    end do
    k=6
    do i=1,jori
      v=abs(oviol(i))
      if (indiv) vori(ioviol(i),n)=v
      if (v.gt.cut(k)) ivio(k)=ivio(k)+1
      vsum(k)=vsum(k)+v**modexp
      vmax(k)=max(vmax(k),v)
    end do
    k=7
    do i=1,ndip ! jpsevio. ora glieli facciamo scrivere tutti
      v=abs(pviol(i))
      if (indiv) vpse(i,n)=v ! vpse(ioviol(i),n)=v
      if (v.gt.cut(k)) ivio(k)=ivio(k)+1
      vsum(k)=vsum(k)+v**modexp
      vmax(k)=max(vmax(k),v)
    end do
    do i=1,ntyp
      k=ityp(i)
      vsum(k)=vsum(k)/ncon(k)
      if (mode.eq.3 .and. k.ne.3) vsum(k)=sqrt(max(zero,vsum(k)))
      write (line(len_trim(line)+1:),fmt(k)) ivio(k),vsum(k),vmax
      iviosu(k)=iviosu(k)+ivio(k)
      vsumsu(k)=vsumsu(k)+vsum(k)
      vmaxsu(k)=vmaxsu(k)+vmax(k)
      iviosq(k)=iviosq(k)+ivio(k)**2
      vsumsq(k)=vsumsq(k)+vsum(k)**2
```

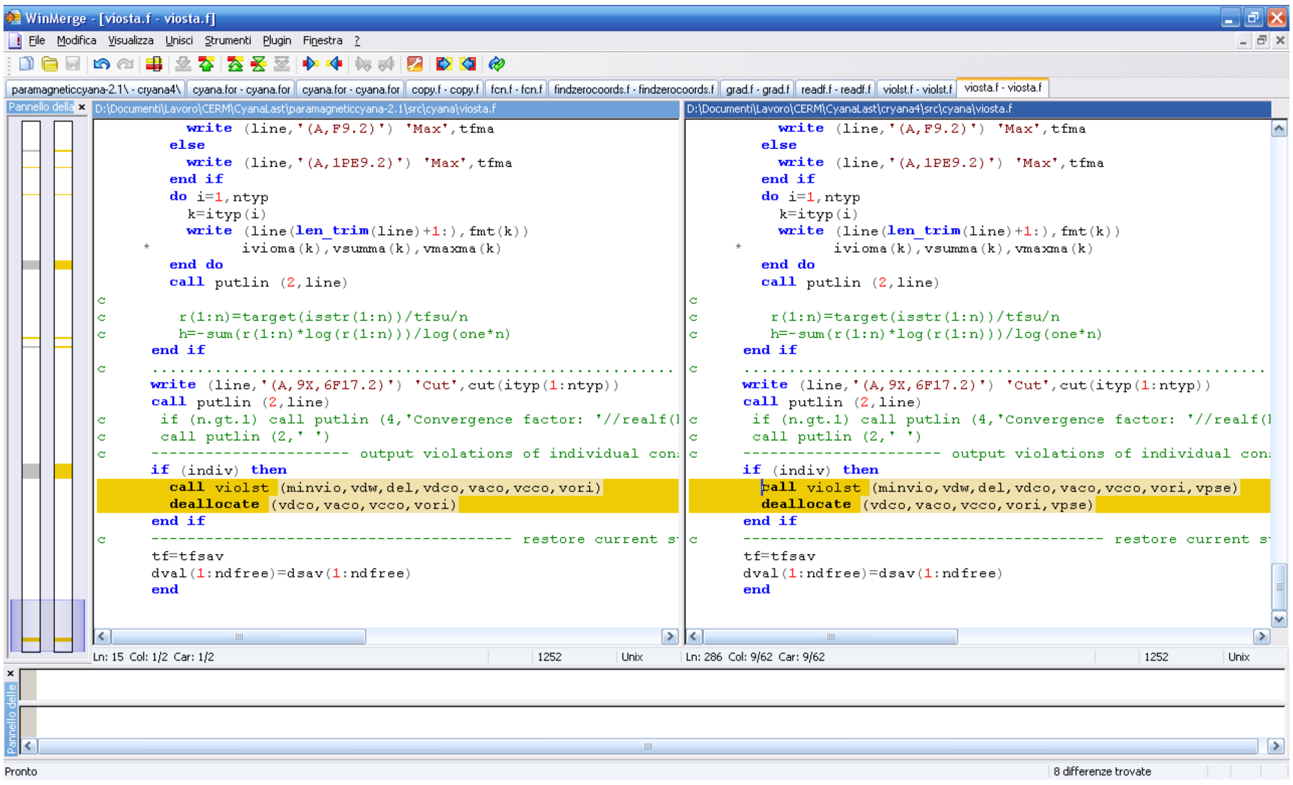
Ln: 189 Col: 15/15 Car: 15/15 1252 Unix

8) change

```
call violst (minvio,vdw,del,vdco,vaco,vcco,vori)
deallocate (vdco,vaco,vcco,vori)
```

→

```
call violst (minvio,vdw,del,vdco,vaco,vcco,vori,vpse)
deallocate (vdco,vaco,vcco,vori,vpse)
```


WinMerge - [viosta.f - viosta.f]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\viosta.f

```
            write (line,'(A,F9.2)') 'Max',tfma
          else
            write (line,'(A,1PE9.2)') 'Max',tfma
          end if
          do i=1,ntyp
            k=ityp(i)
            write (line(len_trim(line)+1:),fmt(k))
     *            ivioma(k),vsumma(k),vmaxma(k)
          end do
          call putlin (2,line)
c
c          r(1:n)=target(isstr(1:n))/tfsu/n
c          h=-sum(r(1:n)*log(r(1:n)))/log(one*n)
        end if
c       ..........................................................
        write (line,'(A,9X,6F17.2)') 'Cut',cut(ityp(1:ntyp))
        call putlin (2,line)
c        if (n.gt.1) call putlin (4,'Convergence factor: '//realf(l
c        call putlin (2,' ')
c       ---------------------- output violations of individual con:
        if (indiv) then
          call violst (minvio,vdw,del,vdco,vaco,vcco,vori)
          deallocate (vdco,vaco,vcco,vori)
        end if
c       ---------------------------------------- restore current s
        tf=tfsav
        dval(1:ndfree)=dsav(1:ndfree)
        end
```

Ln: 15 Col: 1/2 Car: 1/2 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\viosta.f

```
            write (line,'(A,F9.2)') 'Max',tfma
          else
            write (line,'(A,1PE9.2)') 'Max',tfma
          end if
          do i=1,ntyp
            k=ityp(i)
            write (line(len_trim(line)+1:),fmt(k))
     *            ivioma(k),vsumma(k),vmaxma(k)
          end do
          call putlin (2,line)
c
c          r(1:n)=target(isstr(1:n))/tfsu/n
c          h=-sum(r(1:n)*log(r(1:n)))/log(one*n)
        end if
c       ..........................................................
        write (line,'(A,9X,6F17.2)') 'Cut',cut(ityp(1:ntyp))
        call putlin (2,line)
c        if (n.gt.1) call putlin (4,'Convergence factor: '//realf(l
c        call putlin (2,' ')
c       ---------------------- output violations of individual con:
        if (indiv) then
          call violst (minvio,vdw,del,vdco,vaco,vcco,vori,vpse)
          deallocate (vdco,vaco,vcco,vori,vpse)
        end if
c       ---------------------------------------- restore current s
        tf=tfsav
        dval(1:ndfree)=dsav(1:ndfree)
        end
```

Ln: 286 Col: 9/62 Car: 9/62 1252 Unix

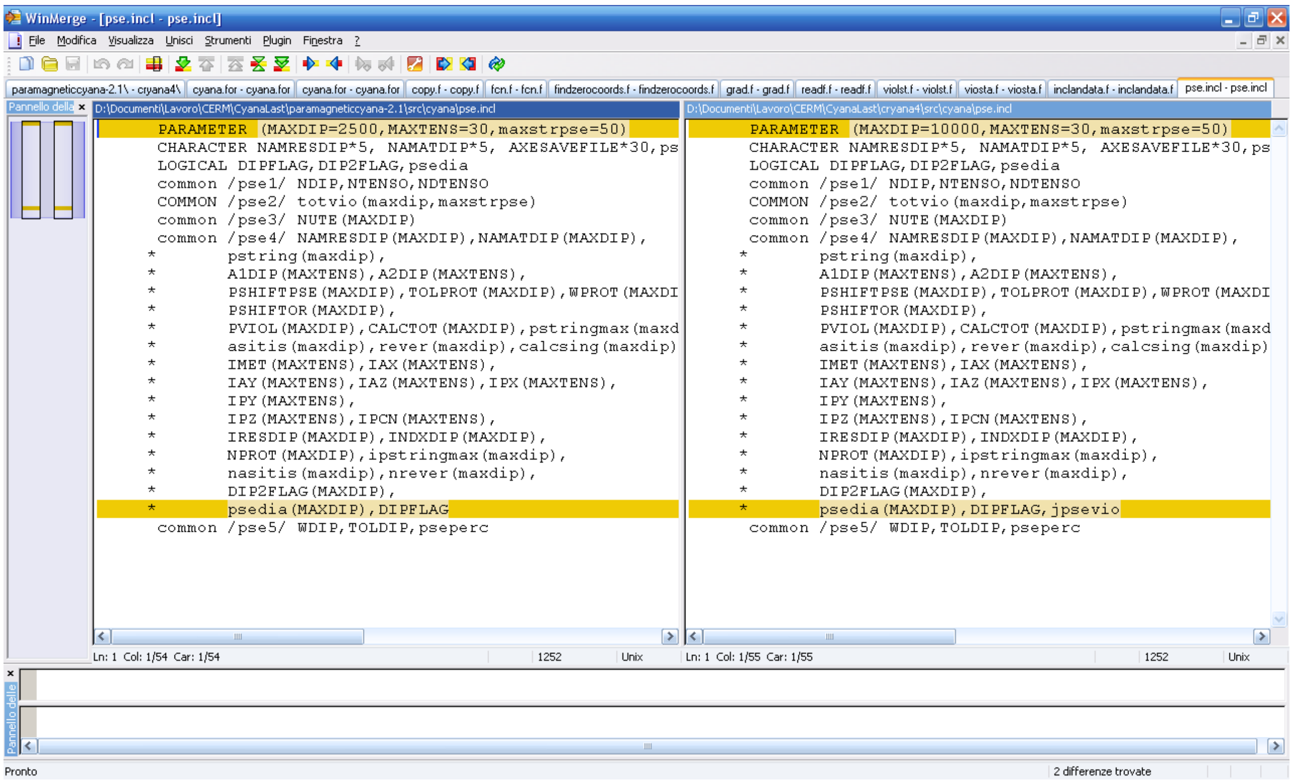
Pronto 8 differenze trovate

pse.incl

1) change

`MAXDIP=2500` → `MAXDIP=10000`

2) add variable `jpsevio`


WinMerge - [pse.incl - pse.incl]

D:\Documenti\Lavoro\CERM\CyanaLast\paramagneticcyana-2.1\src\cyana\pse.incl

```
      PARAMETER (MAXDIP=2500,MAXTENS=30,maxstrpse=50)
      CHARACTER NAMRESDIP*5, NAMATDIP*5, AXESAVEFILE*30,ps
      LOGICAL DIPFLAG,DIP2FLAG,psedia
      common /pse1/ NDIP,NTENSO,NDTENSO
      COMMON /pse2/ totvio(maxdip,maxstrpse)
      common /pse3/ NUTE(MAXDIP)
      common /pse4/ NAMRESDIP(MAXDIP),NAMATDIP(MAXDIP),
     *        pstring(maxdip),
     *        A1DIP(MAXTENS),A2DIP(MAXTENS),
     *        PSHIFTPSE(MAXDIP),TOLPROT(MAXDIP),WPROT(MAXDI
     *        PSHIFTOR(MAXDIP),
     *        PVIOL(MAXDIP),CALCTOT(MAXDIP),pstringmax(maxd
     *        asitis(maxdip),rever(maxdip),calcsing(maxdip)
     *        IMET(MAXTENS),IAX(MAXTENS),
     *        IAY(MAXTENS),IAZ(MAXTENS),IPX(MAXTENS),
     *        IPY(MAXTENS),
     *        IPZ(MAXTENS),IPCN(MAXTENS),
     *        IRESDIP(MAXDIP),INDXDIP(MAXDIP),
     *        NPROT(MAXDIP),ipstringmax(maxdip),
     *        nasitis(maxdip),nrever(maxdip),
     *        DIP2FLAG(MAXDIP),
     *        psedia(MAXDIP),DIPFLAG
      common /pse5/ WDIP,TOLDIP,pseperc
```

Ln: 1 Col: 1/54 Car: 1/54 1252 Unix

D:\Documenti\Lavoro\CERM\CyanaLast\cryana4\src\cyana\pse.incl

```
      PARAMETER (MAXDIP=10000,MAXTENS=30,maxstrpse=50)
      CHARACTER NAMRESDIP*5, NAMATDIP*5, AXESAVEFILE*30,ps
      LOGICAL DIPFLAG,DIP2FLAG,psedia
      common /pse1/ NDIP,NTENSO,NDTENSO
      COMMON /pse2/ totvio(maxdip,maxstrpse)
      common /pse3/ NUTE(MAXDIP)
      common /pse4/ NAMRESDIP(MAXDIP),NAMATDIP(MAXDIP),
     *        pstring(maxdip),
     *        A1DIP(MAXTENS),A2DIP(MAXTENS),
     *        PSHIFTPSE(MAXDIP),TOLPROT(MAXDIP),WPROT(MAXDI
     *        PSHIFTOR(MAXDIP),
     *        PVIOL(MAXDIP),CALCTOT(MAXDIP),pstringmax(maxd
     *        asitis(maxdip),rever(maxdip),calcsing(maxdip)
     *        IMET(MAXTENS),IAX(MAXTENS),
     *        IAY(MAXTENS),IAZ(MAXTENS),IPX(MAXTENS),
     *        IPY(MAXTENS),
     *        IPZ(MAXTENS),IPCN(MAXTENS),
     *        IRESDIP(MAXDIP),INDXDIP(MAXDIP),
     *        NPROT(MAXDIP),ipstringmax(maxdip),
     *        nasitis(maxdip),nrever(maxdip),
     *        DIP2FLAG(MAXDIP),
     *        psedia(MAXDIP),DIPFLAG,jpsevio
      common /pse5/ WDIP,TOLDIP,pseperc
```

Ln: 1 Col: 1/55 Car: 1/55 1252 Unix

Pronto 2 differenze trovate

Commands

This section reviews syntax and parameters of the new commands introduced.

To read a `pse` file that is being used considering the contribution to pcs of external symmetric metals, a typical command is the following:

```
read cry observed_pcs.pse tensors=2 weight=0.5 tolerance=0.2 perc=0.2 symmetry=P21212   ↵
         celldimx=69.194 celldimy=62.564 celldimz=37.262
read cos anisoTensor.cos
```

Reading the `cry` file, `tensors` is the number of tensors present in the sequence, including the crystal origin tensor, and they must be specified at the end of the `pse` file (the origin have to be the last tensor in `pse` file).
The symmetry allowed at the moment are P222, P222$_1$, P2$_1$2$_1$2, P2$_1$2$_1$2$_1$.
`celldimx`, `celldimy` and `celldimz` are the dimensions of the asymmetric unit cell.
The meaning of other parameters is obvious.
The `cos` file is the file containing the information of susceptibility magnetic tensor.

If we need to fix a specific orientation for the origin with respect to the metal tensor orientation we can use the following command:

```
read cry observed_pcs.pse tensors=2 weight=0.5 tolerance=0.2 perc=0.2 symmetry=P21212    ↵
         celldimx=69.194 celldimy=62.564 celldimz=37.262 crystal=2 OMweight=100.0
read cos anisoTensor.cos
read omr XY.omr
```

The parameter `crystal=2` (default is `crystal=1`) means that an `omr` file needs to be read to restrain the reciprocal orientation of the two tensors. The `omr` file is just a file containing a matrix. If M is the matrix containing in rows the coordinates of the unit vectors AX, AY and AZ defining the metal tensor orientations and O is the matrix containing in rows the coordinates of the unit vectors defining crystallographic origin orientations, the `omr` file contains the matrix M^TO.

Other useful added commands are:

```
include_cry
exclude_cry
```

to include/exclude the contribution of the global pcs restraints in the calculation of the TF.

An example of pse file

```
155 GLN  C          0.30 1  0.20  1.50  1
155 GLN  CA         0.52 1  0.20  1.50  1
155 GLN  CB         0.30 1  0.20  1.50  1
155 GLN  CG         0.31 1  0.20  1.50  1
155 GLN  CD         0.24 1  0.20  1.50  1
156 SER  C          0.39 1  0.20  1.50  1
156 SER  CA         0.52 1  0.20  1.50  1
156 SER  CB         0.15 1  0.20  1.50  1
157 LEU  C          0.56 1  0.20  1.50  1
157 LEU  CA         0.58 1  0.20  1.50  1
157 LEU  CB         0.81 1  0.20  1.50  1
157 LEU  CG         0.52 1  0.20  1.50  1
200 LTNS ME
40  LTNS ME
```

An example of cos file

```
    1.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    1.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    1.00000E+00
    7.00370E-32   -2.33456E-32
```

The last two numbers of `cos` file are the axial and rhombic components of the susceptibility anisotropy tensor.

An example of omr file

```
    0.78169E+00   -0.39277E+00    0.48486E+00
   -0.55380E+00   -7.92354E-02    0.82870E+00
   -0.28648E+00   -0.91584E+00   -0.28045E+00
```