

## APPENDIX B

# NUMERICAL CODE OF THE CR MODEL

**program CR**

```
implicit none
include 'dati.fi'
include 'parametri_cr.fi'

include 'oggetti.fi'

integer i,iter,ndataaus
double precision fnor(ndatamx)
double precision maxw,dn
external maxw
include 'dati_ar.fi'
include 'valori.fi'
```

c Lettura dei parametri e dei dati iniziali

```
call read_qu
call read_data
call read_data_cr
```

c Calcolo delle particelle totali

```
do i=1,nion_ar
N=N+N_ar(i)
```

end do

c Inizializzazione delle variabili

Te=Te0

c Inizializzazione fdst: Maxwell alla temperatura Te

do i=1,ndata

fdst(i)=maxw(energ(i))

end do

call terminenoto

10 continue

iter=1

20 continue

write(\*,\*)"ITERAZIONE",iter

call discretizzazione

c Inserimento del termine di arricchimento degli integrali di collisione anelastici

call anelastiche

c Soluzione della EEDF

call matrice

call soluzione

do i=1,ndata

fnor(i)=energ(i)\*\*(0.5d0)\*fdst(i)

end do

call trapezi(ndata,energ,fnor,1,nodata,integrale)

write(\*,\*) 'integrale',integrale

c Verifica dei criteri di convergenza della EEDF

```
call convergenza
call temp

if ((diffrel.gt.conv).or.
1      (dabs((Te-Te0)/Te0).gt.convtemp)) then
  if (iter.lt.ritermax) then
    write(*,*)'diffrel',diffrel
    write(*,*)'Te',Te
    Te0=Te
    iter=iter+1
    goto 20
  else
    write(*,*) 'superato limite di iterazioni!',diffrel
    goto 50
  end if
  else
    write(*,*)'ITERAZIONE',iter,'diffrel',diffrel
    write(*,*) 'temperatura',Te
  end if

50 continue
```

c Soluzione del modello CR

```
nk(n_cr+1)=N_ar(3)
call matrix_cr
call soluzione_cr
```

c Verifica dei criteri di convergenza per N\_ar(2)

```
dn=dabs((N_ar(2)-nk(1))/N_ar(2))
if (dn.gt.convN) then
  N_ar(2)=nk(1)
  write(*,*) 'Popolazione ArII',N_ar(2)
  goto 10
else
end if
```

c Calcolo dei parametri di trasporto

```
call zero
call fzerocalc
call funocalc
call drift
call freq
alfa=ni/Vd
```

c Scrittura dei risultati

```
call writeres
call write_nk
```

```
stop
end
```

**subroutine anelastiche**

```
implicit none
include 'oggetti.fi'
include 'dati.fi'
include 'dati_ar.fi'
include 'valori.fi'
```

c Eccitazione e-Ar1 dal livello 1

```
call ter_ecc(necc1_ar1,ndecc1_ar1,qecc1_ar1,N_ar(1),
1              tecc1_ar1,Iecc1_ar1)
```

c Eccitazione e-Ar2 dal livello 1

```
call ter_ecc(necc1_ar2,ndecc1_ar2,qecc1_ar2,N_ar(2),
1              tecc1_ar2,Iecc1_ar2)
```

c Ionizzazione e-Ar dal livello 1

```
call ter_ion(nion_ar,ndion_ar,qion_ar,N_ar,eion_ar,
1              ion_ar,Iion_ar)
```

c Stampa dei termini

```
c      open(unit=10,file='tion_ar.out',status='unknown')
c      do j=1,2*nion_ar
c          write(10,50) j
c          do i=1,ndata
c              write(10,50) i,enereV(i),tion_ar(i,3*j-2),tion_ar(i,3*j-1),
c 1                  tion_ar(i,3*j),lion_ar(i,j)
c          end do
c          end do
c          close (10)

c50      format (i4,g13.5,3g16.8,i6)

c      open(unit=10,file='tecc_ar.out',status='unknown')
c      do j=1,necc1_ar1
c          write(10,50) j
c          do i=1,ndata
c              write(10,50) i,enereV(i),tecc1_ar1(i,3*j-2),tecc1_ar1(i,3*j-1),
c 1                  tecc1_ar1(i,3*j),Iecc1_ar1(i,j)
c          end do
c          end do
c          close (10)

c50      format (i4,g13.5,3g16.8,i6)

      return
end
```

**subroutine convergenza**

```
implicit none
include 'oggetti.fi'
double precision f1,f2,diff
integer i

diffrel=0.d0

do i=1,ndata
f1=fdst0(i)
f2=fdst(i)
if ((f1.eq.0.d0).or.((f1.eq.0.d0).and.(f2.eq.0.d0))) then
```

```

    goto 10
else
    diff=dabs((f1-f2)/f1)
    if (diff.gt.diffrel) then
        diffrel=diff
    else
        end if
    end if
10  continue
    end do

return
end

```

**subroutine deltax(uist,kist,dxist)**

```

implicit none
double precision uist,kist,dxist
include 'oggetti.fi'
include 'dati.fi'
include 'valori.fi'

dxist=2*Kist/Uist

return
end

```

**subroutine discretizzazione**

```

implicit none
integer i,iener,ie,ind,iq
double precision aist,d,uist,kist,dxist,gammaist,p,passo,var
double precision eaus,faus,fint,f1aus,f2aus
include 'oggetti.fi'
double precision maxw,f1(ndatamx),f2(ndatamx)
include 'dati.fi'
include 'valori.fi'

```

c        Inizializzazione delle variabili ausiliarie

```
ndata0=ndata
do i=1,ndata0
    energ0(i)=energ(i)
    fdst0(i)=fdst(i)
    f1(i)=energ0(i)**(1.5d0)*fdst0(i)
    f2(i)=energ0(i)**(0.5d0)*fdst0(i)
end do

c      Inizio della discretizzazione
c      Punto 1

i=1
iq=1
write(*,*) 'discretizzazione in corso.....enereV',enereV(i)
energ(i)=e*enereV(i)
iener=1
ind=1

call trovab
call trovaa(iq,energ(i),aist,d)
    call kappa(f1,energ(i),iener,aist,var,kist)
    call udi(f2,energ(i),iener,aist,d,var,uist)
call gammacalc(f2,energ(i),iener,aist,d,gammaist)
    call deltax(uist,kist,dxist)

A(i)=aist
    DA(i)=d
    U(i)=uist
    K(i)=kist
    dx(i)=dxist
    gamma(i)=gammaist

c      Punti 2,ndata-1

iener=2

do i=2,ndatamx-1

    p=parametro
20        continue
```

```

passo=p*dabs(dx(i-1))

if (i.gt.2) then
    if (passo.gt.2.d0*(energ(i-1)-energ(i-2))) then
        passo=2.d0*(energ(i-1)-energ(i-2))
    else
        end if
    else
        end if
    if (passo.gt.5.d-1*e) then
        passo=5.d-1*e
    else
        end if
    energ(i)=energ(i-1)+passo

do ie=iener,ndata0
    if (energ(i).le.energ0(ie)) then
        iener=ie
        goto 5
    else
        end if
    end do
5      continue

fint=fdst0(iener)-fdst0(iener-1)
fint=fint/(energ0(iener)-energ0(iener-1))
fint=fdst0(iener-1)+fint*(energ(i)-energ0(iener-1))

eaus=energ0(iener)
faus=fdst0(iener)
f1aus=f1(iener)
f2aus=f2(iener)
energ0(iener)=energ(i)
fdst0(iener)=fint
f1(iener)=energ(i)**(1.5d0)*fdst0(iener)
f2(iener)=energ(i)**(0.5d0)*fdst0(iener)

call trovaa(iq,energ(i),aist,d)
call kappa(f1,energ(i),iener,aist,var,kist)
call udi(f2,energ(i),iener,aist,d,var,uist)

```

```
call gammacalc(f2,energ(i),iener,aist,d,gammaist)
call deltax(uist,kist,dxist)

energ0(iener)=eaus
fdst0(iener)=faus
f1(iener)=f1aus
f2(iener)=f2aus

if (dabs(dxist).lt.passo) then
p=parametro*p
goto 20
else
    A(i)=aist
    DA(i)=d
    U(i)=uist
    K(i)=kist
    dx(i)=dxist
    gamma(i)=gammaist
enereV(i)=energ(i)/e
if (enereV(i).gt.enermax) then
    goto 10
else
    end if
end if

end do

10  write (*,*) ' numero di punti ='i

ndata=i

c      Punto ndata

enereV(ndata+1)=enereV(ndata)
enereV(ndata)=enermax
energ(ndata)=enermax*e
energ(ndata+1)=enereV(ndata+1)*e
write(*,*) 'discretizzazione effettuata.....enereV',enereV(ndata)

call trovaa(iq,energ(ndata),aist,d)
```

```

call kappa(f1,energ(ndata),ndata0,aist,var,kist)
call udi(f2,energ(ndata),ndata0,aist,d,var,uist)
call gammacalc(f2,energ(ndata),ndata0,aist,d,gammaist)
call deltax(uist,kist,dxist)

```

```

A(ndata)=aist
DA(ndata)=d
U(ndata)=uist
K(ndata)=kist
dx(ndata)=dxist
gamma(ndata)=gammaist

```

```

c      call salvarisultati
      return
      end

```

### **subroutine drift**

```

implicit none
integer i
include 'oggetti.fi'
double precision faus(ndatamx)
include 'dati.fi'
include 'valori.fi'

Vd=0.d0
do i=1,ndata
faus(i)=energ(i)*funo(i)
end do
call trapezi(ndata,energ,faus,1,ndata,Vd)
Vd=Vd*8.d0*pi/(3.d0*m**2.d0)
Vd=dabs(Vd)

return
end

```

### **subroutine eccdis\_e\_cr(c,f)**

```

c      Questa subroutine calcola gli integrali di collisione:
c      - ecc/disec con elettroni: c/f

```

```
implicit none
include 'parametri_cr.fi'
include 'oggetti.fi'
integer ir,i,j,il,iq,ld
double precision c(n_cr,n_cr),f(n_cr,n_cr)
double precision eh,a0,es,ur,bs,faus,p,q,dp
double precision qu(ndata),qua(ndata),qus(ndata)
double precision a_a,a_p,a_s,x,y,z,ej,a_p1(n_cr)
double precision vaus1(ndatamx),vaus2(ndatamx),eaus(ndatamx)
include 'dati.fi'
include 'dati_ar.fi'
include 'valori.fi'

write(*,*)"Calcolo termini ecc/disec con e'

eh=13.601*e
a0=5.292e-11
bs=1.0d0
a_a=5.0d-1
a_s=2.0d-1
a_p1(17)=1.19d-1
a_p1(18)=8.50d-2
a_p1(19)=1.68d-1
a_p1(20)=5.18d-5
a_p1(21)=2.65d-1
a_p1(22)=8.40d-2
a_p1(23)=5.60d-2
a_p1(24)=1.15d-1
a_p1(25)=8.60d-2
a_p1(26)=1.39d-1
a_p1(27)=3.60d-2
a_p1(30)=3.05d-2
a_p1(31)=1.75d-1
a_p1(32)=1.63d-1
a_p1(33)=1.68d-1
do i=34,n_cr
  a_p1(i)=2.0d-1
end do
```

```
ir=1

do il=ir+1,n_cr

iq=1
es=(elev(il)-elev(ir))*e
do j=1,ndata
if (energ(j).le.es) then
    eaus(j)=energ(j)
    vaus1(j)=0.d0
    vaus2(j)=0.d0
else
    i=j
    eaus(j-1)=es
    goto 10
end if
end do
10   continue
if (fo(ir,il).ne.0.d0) then
    do j=i,ndata
        ur=energ(j)/es
        qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*a_a*ur**(-2.d0)
        qua(j)=qua(j)*(ur-1)*dlog(1.25*bs*ur)
        qus(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
        qu(j)=qua(j)+qus(j)
    end do
else if ((l(ir).ne.10).and.(l(il).ne.10)) then
    ld=abs(l(ir)-l(il))
    if (ld.eq.1) then
        do j=i,ndata
            ur=energ(j)/es
            qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*ur**(-2.d0)
            qua(j)=qua(j)*a_a*(ur-1)*dlog(1.25*bs*ur)
            qus(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
            qu(j)=qua(j)+qus(j)
        end do
    else
        do j=i,ndata
            ur=energ(j)/es
            qu=4*Pi*(a0**2)*a_p1(il)*(1-1/ur)
```

```

        end do
        end if
    else
        p=2*(13.601/(elev(n_cr+1)-elev(ir)))**5.d-1
        q=2*(13.601/(elev(n_cr+1)-elev(il)))**5.d-1
        dp=q-p
        if (y/p.le.1.d0) then
            fo(ir,il)=1.52*p**(-5.d0)*q**(-3.d0)
            fo(ir,il)=fo(ir,il)*((p**(-2.d0)-q**(-2.d0))**(-3.d0))
        else
            fo(ir,il)=1.95*p**(-5.d0)*q**(-3.d0)
            fo(ir,il)=fo(ir,il)*((p**(-2.d0)-q**(-2.d0))**(-3.d0))
        end if
        do j=i,ndata
            ur=energ(j)/es
            qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*ur**(-2.d0)
            qua(j)=qua(j)*a_a*(ur-1)*dlog(1.25*bs*ur)
            quus(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
            qu(j)=qua(j)+quus(j)
        end do
    end if
    do j=i,ndata
        eaus(j)=energ(j)
        vaus1(j)=qu(j)*fdst(j)*eaus(j)
        ej=eaus(j)-es
        call taylor(ndata,energ,ej,iq,x,y,z)
        if (iq.eq.1) then
            faus=fdst(1)*y+fdst(2)*z
        else if (iq.eq.ndata) then
            faus=fdst(ndata-1)*x+fdst(ndata)*y
        else
            faus=fdst(iq-1)*x+fdst(iq)*y+fdst(iq+1)*z
        end if
        vaus2(j)=qu(j)*fAus*eaus(j)
    end do

```

c       Eccitazione

```

call trapezi(ndata,eaus,vaus1,1,ndata,c(ir,il))
c(ir,il)=c(ir,il)*(2.d0/m)**5.d-1

```

## c      Diseccitazione

```
call trapezi(ndata,eaus,vaus2,1,ndata,f(ir,il))
f(ir,il)=f(ir,il)*(2.d0/m)**5.d-1
f(ir,il)=f(ir,il)*g(ir)/(2*g(il))

end do

a_p=2.0d-1

do ir=2,n_cr-1
do il=ir+1,n_cr

    iq=1
    es=(elev(il)-elev(ir))*e
    do j=1,ndata
        if (energ(j).le.es) then
            eaus(j)=energ(j)
            vaus1(j)=0.d0
            vaus2(j)=0.d0
        else
            i=j
            eaus(j-1)=es
            goto 20
        end if
    end do
20    continue
    if (fo(ir,il).ne.0.d0) then
        do j=i,ndata
            ur=energ(j)/es
            qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*a_a*ur**(-2.d0)
            qua(j)=qua(j)*(ur-1)*dlog(1.25*bs*ur)
            qu(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
            qu(j)=qua(j)+qus(j)
        end do
        else if ((l(ir).ne.10).and.(l(il).ne.10)) then
            ld=abs(l(ir)-l(il))
            if (ld.eq.1) then
                do j=i,ndata
```

```

        ur=energ(j)/es
        qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*ur**(-2.d0)
        qua(j)=qua(j)*a_a*(ur-1)*dlog(1.25*bs*ur)
        qus(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
        qu(j)=qua(j)+qus(j)
        end do

        else
        do j=i,ndata
            ur=energ(j)/es
            qu=4*Pi*(a0**2)*a_p*(1-1/ur)
            end do
        end if
        else
        p=2*(13.601/(elev(n_cr+1)-elev(ir)))**5.d-1
        q=2*(13.601/(elev(n_cr+1)-elev(il)))**5.d-1
        dp=q-p
        if (y/p.le.1.d0) then
            fo(ir,il)=1.52*p**(-5.d0)*q**(-3.d0)
            fo(ir,il)=fo(ir,il)*((p**(-2.d0)-q**(-2.d0))**(-3.d0))
        else
            fo(ir,il)=1.95*p**(-5.d0)*q**(-3.d0)
            fo(ir,il)=fo(ir,il)*((p**(-2.d0)-q**(-2.d0))**(-3.d0))
        end if
        if (fo(ir,il).gt.1.d0) then
            write(*,*)'ATTENZIONE fo!!!!',fo(ir,il),ir,il
            fo(ir,il)=fo(ir,il)*5.0d-6
        end if
        do j=i,ndata
            ur=energ(j)/es
            qua(j)=4*Pi*(a0**2)*((eh/es)**2)*fo(ir,il)*ur**(-2.d0)
            qua(j)=qua(j)*a_a*(ur-1)*dlog(1.25*bs*ur)
            qus(j)=4*Pi*(a0**2)*a_s*(1-1/(ur**2))*ur**(-3.d0)
            qu(j)=qua(j)+qus(j)
            end do
        end if

        do j=i,ndata
            eaus(j)=energ(j)
            vaus1(j)=qu(j)*fdst(j)*eaus(j)
            ej=eaus(j)-es
    
```

```

call taylor(ndata,energ,ej,iq,x,y,z)
if (iq.eq.1) then
    faus=fdst(1)*y+fdst(2)*z
else if (iq.eq.ndata) then
    faus=fdst(ndata-1)*x+fdst(ndata)*y
else
    faus=fdst(iq-1)*x+fdst(iq)*y+fdst(iq+1)*z
end if
vaus2(j)=qu(j)*faus*eaus(j)
end do

c      Eccitazione

call trapezi(ndata,eaus,vaus1,1,ndata,c(ir,il))
c(ir,il)=c(ir,il)*(2.d0/m)**5.d-1

c      Diseccitazione

call trapezi(ndata,eaus,vaus2,1,ndata,f(ir,il))
f(ir,il)=f(ir,il)*(2.d0/m)**5.d-1
f(ir,il)=f(ir,il)*g(ir)/(2*g(il))

end do
end do

c      Stampa dei coefficienti

c      open (unit=10,file='c.out',status='unknown')
c      write(10,50) ((c(i,j),j=1,n_cr),i=1,n_cr)
c      close (10)

c      open (unit=10,file='f.out',status='unknown')
c      write(10,50) ((f(i,j),j=1,n_cr),i=1,n_cr)
c      close (10)

c50      format(78e13.4)

return
end

```

**subroutine HAA(i,ai,bi,ci)**

```
    implicit none
    integer i
    double precision isx,idx,ai,bi,ci
    include 'oggetti.fi'

    isx=energ(i)-energ(i-1)
    idx=energ(i+1)-energ(i)

    ai=1.d0/(isx*(isx+idx))*(2.d0-U(i)/K(i)*idx)
    bi=-1.d0/(isx*idx)*(2.d0+U(i)/K(i)*(isx-idx)-gamma(i)/K(i)*isx*idx)
    ci=1.d0/(idx*(isx+idx))*(2+U(i)/K(i)*isx)

    return
    end
```

**subroutine emisspont\_cr(ac)**

c Questa subroutine calcola gli integrali di collisione:  
c - emissione spontanea: ac

```
    implicit none
    integer ir,il
    include 'parametri_cr.fi'
    include 'oggetti.fi'
    double precision ac(n_cr,n_cr),es
    include 'dati.fi'
    include 'dati_ar.fi'
    include 'valori.fi'

    write(*,*)"Calcolo termini di emissione spontanea"
```

```
    do ir=1,n_cr-1
        do il=ir+1,n_cr
            es=(elev(il)-elev(ir))*e
            ac(ir,il)=fo(ir,il)*(es**2)*g(ir)/g(il)
            ac(ir,il)=ac(ir,il)/(1.5d0*(h*cl*1.0d2)**2)
        end do
    end do
```

```
    return  
    end
```

**subroutine freq**

```
implicit none  
integer i,j,ii,iq  
include 'oggetti.fi'  
double precision mu(10),vaus(ndatamx)  
double precision qu,x,y,z  
include 'dati.fi'  
include 'dati_ar.fi'  
include 'valori.fi'  
  
ni=0.d0  
do ii=1,nion_ar  
    iq=1  
    do j=1,ndion_ar(ii)  
        x0(j)=qion_ar(j,2*ii-1)  
        f0(j)=qion_ar(j,2*ii)  
    end do  
    mu(ii)=0.d0  
    do i=1,ndata  
        if (energ(i).le.eion_ar(ii)) then  
            qu=0.d0  
        else  
            call taylor(ndion_ar(ii),x0,energ(i),iq,x,y,z)  
            if (iq.eq.1) then  
                qu=f0(1)*y+f0(2)*z  
            else if (iq.eq.ndion_ar(ii)) then  
                qu=f0(ndion_ar(ii)-1)*x+f0(ndion_ar(ii))*y  
            else  
                qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z  
            end if  
        end if  
        if (qu.lt.0.d0) then  
            write(*,*) 'XXXXXXXXXXXXXXXXXXXXXXXXXXXX'  
        else  
        end if
```

```
    vaus(i)=qu*fzero(i)*energ(i)
end do
call trapezi(ndata,energ,vaus,1,ndata,mu(ii))
mu(ii)=8.d0*Pi*N_ar(ii)*mu(ii)/(m*m)
end do

do i=1,nion_ar
ni=ni+mu(i)
end do

return
end
```

**subroutine funocalc**

```
implicit none
include 'dati.fi'
include 'oggetti.fi'
integer i
double precision caus
include 'valori.fi'

caus=e*campo

do i=1,ndata
funo(i)=caus*dfzero(i)/A(i)-alfa*fzero(i)/A(i)
end do

return
end
```

**subroutine fzerocalc**

C\*\*\*\*\*calcolo fzero e la sua derivata rispetto alla energia\*\*\*\*\*

```
implicit none
include 'dati.fi'
include 'oggetti.fi'
double precision a1
double precision denerdx,denersx,dener
```

```
integer i
include 'valori.fi'

a1=4.d0*Pi*dsqrt(2.d0)/m**1.5d0

do i=1,ndata
    fzero(i)=fdst(i)/a1
end do

c      Derivata dfzero numerica

dfzero(1)=(fzero(2)-fzero(1))/(energ(2)-energ(1))
do i=2,ndata-1
    denerdx=energ(i+1)-energ(i)
    denersx=energ(i)-energ(i-1)
    dener=denerdx+denersx
    dfzero(i)=(fzero(i+1)-fzero(i))*denersx/(denerdx*dener) +
1      (fzero(i)-fzero(i-1))*denerdx/(denersx*dener)
end do
dfzero(ndata)=(fzero(ndata)-fzero(ndata-1))
1/(energ(ndata)-energ(ndata-1))

return
end
```

**subroutine gammacalc(f,ener,ien,aist,d,gammaist)**

```
implicit none
double precision caus1,caus2,caus3,ener,aist,d,gammaist
double precision vaus1,vaus2,vaus3,vaus4,vaus5
integer i,j,ien,iq
double precision qu,x,y,z
include 'dati.fi'
include 'oggetti.fi'
double precision f(ndatamx)
include 'dati_ar.fi'
include 'valori.fi'

caus1=(2.d0/3.d0)*alfa*e*campo/m**2.d0
caus2=-(2.d0/3.d0)*(alfa/m)**2.d0
```

```

caus3=-4.d0/(m*m_ar)

vaus1=caus1*(1.d0/aist-(ener/aist**2.d0)*d)
vaus2=caus2*ener/aist
vaus3=caus3*(2.d0*ener*aist+ener*ener*d)

c      Contributo di Fokker-Plank

vaus4=-f(ien)*B

c      Somma dei contributi

gammaist=vaus1+vaus2+vaus3+vaus4

c      Termine di impoverimento della ionizzazione dell'Argon

do i=1,nion_ar
    iq=1
    do j=1,ndion_ar(i)
        x0(j)=qion_ar(j,2*i-1)
        f0(j)=qion_ar(j,2*i)
    end do
    if (ener.le.eion_ar(i)) then
        qu=0.d0
    else
        call taylor(ndion_ar(i),x0,ener,iq,x,y,z)
        if (iq.eq.1) then
            qu=f0(1)*y+f0(2)*z
        else if (iq.eq.ndion_ar(i)) then
            qu=f0(ndion_ar(i)-1)*x+f0(ndion_ar(i))*y
        else
            qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z
        end if
    end if
    if (qu.lt.0.d0) then
        write(*,*) 'gamma.f_ion',qu,i,ener
    else
        end if
    vaus5=qu*2.d0*N_ar(i)/(m*m)*ener
    gammaist=gammaist+vaus5

```

end do

c Termine di impoverimento dell'eccitazione dell'ArI

```

vaus5=0.d0
do i=1,necc1_ar1
    iq=1
    do j=1,ndecc1_ar1(i)
        x0(j)=qecc1_ar1(j,2*i-1)
        f0(j)=qecc1_ar1(j,2*i)
    end do
    if (ener.le.qecc1_ar1(1,2*i-1)) then
        qu=0.d0
    else
        call taylor(ndecc1_ar1(i),x0,ener,iq,x,y,z)
        if (iq.eq.1) then
            qu=f0(1)*y+f0(2)*z
        else if (iq.eq.ndecc1_ar1(i)) then
            qu=f0(ndecc1_ar1(i)-1)*x+f0(ndecc1_ar1(i))*y
        else
            qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z
        end if
    end if
    if (qu.lt.0.d0) then
        write(*,*) 'gamma.f_ecc_Ar1',qu,i,ener
    else
        end if
        vaus5=qu*2.d0*N_ar1/(m*m)*ener
        gammaist=gammaist+vaus5
    end do

```

c Termine di impoverimento dell'eccitazione dell'ArII

```

vaus5=0.d0
do i=1,necc1_ar2
    iq=1
    do j=1,ndecc1_ar2(i)
        x0(j)=qecc1_ar2(j,2*i-1)
        f0(j)=qecc1_ar2(j,2*i)
    end do

```

```

if (ener.le.qecc1_ar2(1,2*i-1)) then
    qu=0.d0
else
    call taylor(ndecc1_ar2(i),x0,ener,iq,x,y,z)
    if (iq.eq.1) then
        qu=f0(1)*y+f0(2)*z
    else if (iq.eq.ndecc1_ar2(i)) then
        qu=f0(ndecc1_ar2(i)-1)*x+f0(ndecc1_ar2(i))*y
    else
        qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z
    end if
end if
if (qu.lt.0.d0) then
    write(*,*) 'gamma.f_ecc_Ar2',qu,i,ener
else
end if
vaus5=qu*2.d0*N_ar2/(m*m)*ener
gammaist=gammaist+vaus5
end do

return
end

```

**subroutine intnorm**

```

implicit none
double precision mu
include 'oggetti.fi'
integer i

integrale=0.d0
do i=2,ndata
    mu=fdst(i-1)*dsqrt(energ(i-1))+fdst(i)*dsqrt(energ(i))
    mu=mu*(energ(i)-energ(i-1))/2.d0
    integrale=integrale+mu
end do

return
end

```

**subroutine ionric\_e\_cr(s,q)**

- c Questa subroutine calcola gli integrali di collisione:  
c - ioniz/ricom con elettroni: s/o

```
implicit none
integer i,j,iq,ir,iel
include 'parametri_cr.fi'
include 'oggetti.fi'
double precision es,faus,a1,b1,eh,a0,ur
double precision vaus1(ndatamx),vaus2(ndatamx),eaus(ndatamx)
double precision qu,x,y,z,ej
double precision s(n_cr),q(n_cr)
include 'dati.fi'
include 'dati_ar.fi'
include 'valori.fi'

write(*,*)"Calcolo termini ioniz/ricom con e"

eh=13.601*e
a0=5.292e-11
do j=1,ndion_ar(2)
  x0(j)=qion_ar(j,2*2-1)
  f0(j)=qion_ar(j,2*2)
end do
iel=1

do ir=1,n_cr
  iq=1
  es=(elev(n_cr+1)-elev(ir))*e
  do j=1,ndata
    if (energ(j).le.es) then
      eaus(j)=energ(j)
      vaus1(j)=0.d0
      vaus2(j)=0.d0
    else
      i=j
      eaus(j-1)=es
      goto 10
    end if
  end do
end do
```

```

        end do
10      continue
        do j=i,ndata
            eaus(j)=energ(j)
            ur=eaus(j)/es
            if (ir.eq.1) then
                a1=3.5d-1
                b1=1.5
            else if (ir.le.37) then
                a1=4.0d-1
                b1=4.0
            else
                a1=6.7d-1
                b1=1.0
            end if
            qu=4*Pi*(a0**2)*((eh/es)**2)*iel*a1*ur**(-2.d0)
            qu=qu*(ur-1)*dlog(1.25*b1*ur)
            vaus1(j)=qu*fdst(j)*eaus(j)
            ej=eaus(j)-es
            call taylor(ndata,energ,ej,iq,x,y,z)
            if (iq.eq.1) then
                faus=fdst(1)*y+fdst(2)*z
            else if (iq.eq.ndata) then
                faus=fdst(ndata-1)*x+fdst(ndata)*y
            else
                faus=fdst(iq-1)*x+fdst(iq)*y+fdst(iq+1)*z
            end if
            vaus2(j)=qu*faus*eaus(j)
        end do
    
```

c        Ionizzazione

```

call trapezi(ndata,eaus,vaus1,1,ndata,s(ir))
s(ir)=s(ir)*(2.d0/m)**5.d-1
    
```

c        Ricombinazione

```

call trapezi(ndata,eaus,vaus2,1,ndata,q(ir))
q(ir)=q(ir)*(2.d0/m)**5.d-1
q(ir)=q(ir)*g(ir)/(2*g(n_cr+1))
    
```

```
q(ir)=q(ir)*((h*h)/(2*Pi*m*kboltz*Te))**1.5d0
```

```
end do
```

```
return
```

```
end
```

**subroutine kappa(fa,ener,ien,aist,var,kist)**

```
implicit none
```

```
integer i,ien
```

```
include 'dati.fi'
```

```
include 'oggetti.fi'
```

```
double precision var1,var2,var,vaus1,vaus2,vaus3,ener,aist,kist
```

```
double precision fa(ndatamx)
```

```
include 'dati_ar.fi'
```

```
include 'valori.fi'
```

```
vaus1=-(2.d0/3.d0)*(e*campo/m)**2.d0*ener/aist
```

```
vaus2=-kboltz*Th/(m*m_ar)*aist*4.d0*ener*ener
```

c Contributo di Fokker-Plank

```
if (ien.eq.1) then
```

```
var1=0.d0
```

```
else
```

```
call trapezi(ndata0,energ0,fa,1,ien,var1)
```

```
end if
```

```
if (ien.eq.ndata0) then
```

```
var2=0.d0
```

```
else
```

```
call trapezi(ndata0,energ0,fdst0,ien,ndata0,var)
```

```
var2=var*energ0(ien)**(1.5d0)
```

```
end if
```

```
vaus3=(-2.d0/3.d0)*B*(var1+var2)
```

c Somma totale dei contributi

```
kist=vaus1+vaus2+vaus3
```

```
return  
end
```

**subroutine matrice**

```
implicit none  
integer i,j,jj,iaus,g,ik,icont,ntot  
integer min,jtemp  
parameter (icont=100)  
integer jaus(cont)  
double precision elem1,elem2,elem3,atemp  
double precision aaus(cont)  
include 'dati.fi'  
include 'oggetti.fi'  
include 'dati_ar.fi'  
include 'valori.fi'
```

c Gli elementi della matrice sono memorizzati nei seguenti vettori:  
c AA vettore degli elementi non nulli  
c IA indice di riga  
c JA indice di colonna  
c Gli elementi sono memorizzati riga per riga

```
do i=1,ndatamx  
AA(i)=0.d0  
IA(i)=0  
JA(i)=0  
end do
```

c Numero dei processi anelastici totali considerati

```
ntot=necc1_ar1+necc1_ar2+2*nion_ar
```

c La prima riga della matrice contiene la condizione di normalizzazione

```
AA(1)=5.d-1*dsqrt(energ(1))*(energ(2)-energ(1))  
IA(1)=1  
JA(1)=1  
do i=2,ndata-1  
AA(i)=5.d-1*dsqrt(energ(i))*(energ(i+1)-energ(i-1))
```

```

IA(i)=1
JA(i)=i
end do
AA(ndata)=5.d-1*dsqrt(energ(ndata))*(energ(ndata)-energ(ndata-1))
IA(ndata)=1
JA(ndata)=ndata

```

c Inserimento dei coefficienti della matrice da 2 a ndata-1

```

iaus=ndata
iaus=iaus+1

```

```
do i=2,ndata-1
```

c Inserimento dei termini della diagonale principale e delle 2 co-diagonali

```

call HAA(i,elem1,elem2,elem3)
AA(iaus)=elem1
IA(iaus)=i
JA(iaus)=i-1
iaus=iaus+1
AA(iaus)=elem2
IA(iaus)=i
JA(iaus)=i
iaus=iaus+1
AA(iaus)=elem3
IA(iaus)=i
JA(iaus)=i+1

```

c Inserimento dei termini di arricchimento delle collisioni anelastiche

```

iaus=iaus+1
ik=1
do j=1,3*ntot
    aaus(j)=0.d0
    jaus(j)=0
end do

```

c Eccitazione e-ArI

```
do j=1,necc1_ar1
    g=Iecc1_ar1(i,j)
    if (g.ne.0) then
        aaus(ik)=tecc1_ar1(i,3*j-2)
        jaus(ik)=g-1
        ik=ik+1
        aaus(ik)=tecc1_ar1(i,3*j-1)
        jaus(ik)=g
        ik=ik+1
        if (g.eq.ndata) then
            continue
        else
            aaus(ik)=tecc1_ar1(i,3*j)
            jaus(ik)=g+1
            ik=ik+1
        end if
        else
            goto 10
        end if
    end do
10      continue
```

c       Eccitazione e-ArII

```
do j=1,necc1_ar2
    g=Iecc1_ar2(i,j)
    if (g.ne.0) then
        aaus(ik)=tecc1_ar2(i,3*j-2)
        jaus(ik)=g-1
        ik=ik+1
        aaus(ik)=tecc1_ar2(i,3*j-1)
        jaus(ik)=g
        ik=ik+1
        if (g.eq.ndata) then
            continue
        else
            aaus(ik)=tecc1_ar2(i,3*j)
            jaus(ik)=g+1
            ik=ik+1
        end if
```

```

        else
            goto 20
        end if
    end do
20      continue

c      Ionizzazioni e-Ar

do j=1,2*nion_ar
    g=Iion_ar(i,j)
    if (g.ne.0) then
        aaus(ik)=tion_ar(i,3*j-2)
        jaus(ik)=g-1
        ik=ik+1
        aaus(ik)=tion_ar(i,3*j-1)
        jaus(ik)=g
        ik=ik+1
        if (g.eq.ndata) then
            continue
        else
            aaus(ik)=tion_ar(i,3*j)
            jaus(ik)=g+1
            ik=ik+1
        end if
        else
            goto 30
    end if
end do
30      continue

```

c      Ordinamento crescente del vettore aaus in base all'indice di colonna jaus

```

do jj=1,ik-2
    min=jj
    do j=jj+1,ik-1
        if (jaus(j).lt.jaus(min)) then
            min=j
        end if
    end do
    if (min.gt.jj) then

```

```

jtemp=jaus(min)
atemp=aaus(min)
jaus(min)=jaus(jj)
aaus(min)=aaus(jj)
jaus(jj)=jtemp
aaus(jj)=atemp
else
end if
end do

```

c Costruisco il vettore AA sommando i termini che hanno l'indice di colonna comune

```

do ik=1,3*ntot
    if (jaus(ik).ne.0) then
        AA(iaus)=aaus(ik)
        IA(iaus)=i
        JA(iaus)=jaus(ik)
        do j=ik+1,3*ntot
            if (jaus(j).eq.jaus(ik)) then
                AA(iaus)=AA(iaus)+aaus(j)
                jaus(j)=0
            else
            end if
        end do
        iaus=iaus+1
        goto 40
    else
    end if
40      continue
end do

```

end do

c Ultima riga

```

call HAA(ndata,elem1,elem2,elem3)
AA(iaus)=elem1
IA(iaus)=ndata
JA(iaus)=ndata-1
iaus=iaus+1

```

```
AA(iaus)=elem2
IA(iaus)=ndata
JA(iaus)=ndata

nzero=iaus

c      Stampa dei vettori

c      open (unit=10,file='matrix.out',status='unknown')
c      write(10,48) 'elementi non nulli = ',nzero
c      write(10,49) 'IA','JA','AA'
c      do i=1,nzero
c          write(10,50) IA(i),JA(i),AA(i)
c      end do
c      close (10)

c148   format(a20,i6)
c149   format(2a6,a14)
c150   format(2i6,g16.8)

return
end
```

**subroutine matrix\_cr**

```
implicit none
integer i,j,k
include 'parametri_cr.fi'
include 'dati.fi'
double precision aus1,aus2,aus3
double precision ac(n_cr,n_cr),la(n_cr,n_cr),c(n_cr,n_cr)
double precision s(n_cr),q(n_cr),lr(n_cr),r(n_cr),f(n_cr,n_cr)

c      Gli elementi della matrice sono memorizzati nei seguenti vettori:
c      a_cr      vettore degli elementi non nulli
c      Ia_cr     indice di riga
c      Ja_cr     indice di colonna

c      Inizializzazione delle variabili
```

```

do i=1,n_cr
do j=1,n_cr
    a_cr(i,j)=0.d0
end do
end do

do i=1,n_cr
    lr(i)=1
    sc_cr=0.d0
end do

do i=1,n_cr
    do j=1,n_cr
        la(i,j)=1
    end do
end do

alfa_cr=0.d0
s_cr=0.d0

c      Calcolo degli integrali di collisione

call ionric_e_cr(s,q)
call ricrad_cr(r)
call eccdis_e_cr(c,f)
call emisspont_cr(ac)

write(*,*)"Calcolo matrice"

c      Prima riga: condizione di neutralità del plasma

do j=1,n_cr
    a_cr(1,j)=1
end do

c      Righe 2-n_cr: rate equations

do k=2,n_cr

    do j=1,k-1

```

## APPENDIX B

---

```
a_cr(k,j)=ne*c(j,k)
end do

aus1=0.d0
aus2=0.d0
do j=1,k-1
aus1=aus1+ne*f(j,k)+ac(j,k)*la(j,k)
end do
do j=k+1,n_cr
aus2=aus2+ne*c(k,j)
end do
aus3=ne*s(k)
a_cr(k,k)=-(aus1+aus2+aus3)
```

```
do j=k+1,n_cr
a_cr(k,j)=ne*f(k,j)+ac(k,j)*la(k,j)
end do
```

```
end do
```

c Termine noto

```
tn_cr(1)=ne-2*nk(n_cr+1)
do k=2,n_cr
tn_cr(k)=-nk(n_cr+1)*(ne*ne*q(k)+ne*lr(k)*r(k))
end do
```

c Calcolo di alfa\_cr e sc\_cr

```
do j=1,n_cr
alfa_cr=alfa_cr+ne*q(j)+lr(j)*r(j)
sc_cr(j)=ne*s(j)
end do
alfa_cr=ne*nk(n_cr+1)*alfa_cr
```

c Stampa della matrice

```
c open (unit=10,file='matrix_cr.out',status='unknown')
c write(10,50) ((a_cr(i,j),j=1,n_cr+1),i=1,n_cr+1)
c close (10)
```

```
c50      format(79e13.4)

return
end

double precision function maxw(x)

implicit none
double precision x
include 'dati.fi'

costmaxw=2.d0/(dsqrt(Pi)*(kboltz*Te)**1.5d0)
maxw=costmaxw*dexp(-x/(kboltz*Te))

return
end

subroutine read_qu

implicit none
integer i,j
include 'dati.fi'
include 'oggetti.fi'
include 'dati_ar.fi'

c      Lettura delle sezioni d'urto momentum transfer e-ArI

open(unit=10,file='qel-ar.txt',status='old',readonly)
read(10,*) ndel_ar
do j=1,ndel_ar
    read(10,*) qel_ar(j,1),qel_ar(j,2)
    qel_ar(j,1)=qel_ar(j,1)*e
    qel_ar(j,2)=qel_ar(j,2)*1.d-20
end do

c      Lettura di tutte le sezioni d'urto di ionizzazione e-Ar: 1-i

open (unit=10,file='qion-ar.txt',status='old',readonly)
read(10,*) nion_ar
```

```
do i=1,nion_ar
  read(10,*) ndion_ar(i)
    do j=1,ndion_ar(i)
      read(10,*) qion_ar(j,2*i-1),qion_ar(j,2*i)
      qion_ar(j,2*i-1)=qion_ar(j,2*i-1)*e
      qion_ar(j,2*i)=qion_ar(j,2*i)*1.d-20
    end do
  end do
close (10)
```

c Lettura delle sezioni d'urto di eccitazione e-ArI: 1-n

```
open (unit=10,file='qecc1-ar1.txt',status='old',readonly)
read(10,*) necc1_ar1
do i=1,necc1_ar1
  read(10,*) ndecc1_ar1(i)
    do j=1,ndecc1_ar1(i)
      read(10,*) qecc1_ar1(j,2*i-1),qecc1_ar1(j,2*i)
      qecc1_ar1(j,2*i-1)=qecc1_ar1(j,2*i-1)*e
      qecc1_ar1(j,2*i)=qecc1_ar1(j,2*i)*1.d-20
    end do
  end do
close (10)
```

c Lettura delle sezioni d'urto di eccitazione e-ArII: 1-n

```
open (unit=10,file='qecc1-ar2.txt',status='old',readonly)
read(10,*) necc1_ar2
do i=1,necc1_ar2
  read(10,*) ndecc1_ar2(i)
    do j=1,ndecc1_ar2(i)
      read(10,*) qecc1_ar2(j,2*i-1),qecc1_ar2(j,2*i)
      qecc1_ar2(j,2*i-1)=qecc1_ar2(j,2*i-1)*e
      qecc1_ar2(j,2*i)=qecc1_ar2(j,2*i)*1.d-20
    end do
  end do
close (10)
```

```
return
end
```

**subroutine read\_data**

```
implicit none
integer i,j
include 'dati.fi'
include 'oggetti.fi'
include 'dati_ar.fi'

c      Lettura dei parametri di ingresso

open (unit=10,file='dati.txt',status='old',readonly)
read(10,*) Te0
read(10,*) Th
read(10,*) campo
read(10,*) Ne
do i=1,nion_ar
  read(10,*) N_ar(i)
end do
close (10)

c      Lettura del vettore iniziale delle energie [J]

open(unit=10,file='fdata.txt',status='old',readonly)
read (10,*) ndata
do i=1,ndata
  read(10,*) energ(i)
end do
close(10)

return
end
```

**subroutine read\_data\_cr**

```
implicit none
integer i,j
include 'parametri_cr.fi'
include 'oggetti.fi'
include 'dati.fi'
```

```

include 'valori.fi'

c      Lettura dei dati dei livelli energetici

open (unit=10,file='dati_liv.txt',status='old',readonly)
do i=1,n_cr+1
    read(10,*) elev(i),g(i),l(i)
end do
close (10)

c      Lettura della f osc

open (unit=10,file='freq_osc.txt',status='old',readonly)
do i=1,n_cr-1
    do j=i+1,n_cr
        read(10,*) fo(i,j)
    end do
end do
close (10)

return
end

subroutine ricrad_cr(r)

c      Questa subroutine calcola gli integrali di collisione:
c      - ricombinazione radiativa: r

implicit none
integer ir,j,i,iq
include 'oggetti.fi'
include 'parametri_cr.fi'
double precision x,y,z,ej,es,faus,eh
double precision r(n_cr),vaus(ndatamx),eaus(ndatamx)
double precision qu(ndatamx)
include 'dati.fi'
include 'valori.fi'

write(*,*)"Calcolo termini di ricombinazione radiativi"

```

```
eh=13.601*e
do ir=1,n_cr
  es=(elev(n_cr+1)-elev(ir))*e
  do j=1,ndata
    if (energ(j).le.es) then
      eaus(j)=energ(j)
      vaus(j)=0.d0
    else
      i=j
      eaus(j-1)=es
      goto 10
    end if
  end do
10  continue
  if (ir.eq.1) then
    do j=i,ndata
      if (energ(j).le.2*eh) then
        qu(j)=3.5d-21
      else
        qu(j)=2.8d-20*(eh/energ(j))**3
      end if
    end do
    else if (ir.ge.2.and.ir.le.16) then
      do j=i,ndata
        if (energ(j).le.5.9d-1*eh) then
          qu(j)=2.0d-22*0.06
        else
          qu(j)=7.91d-22*0.06*((es/eh)**2.5d0)*(eh/energ(j))**3
        end if
      end do
    else
      do j=i,ndata
        qu(j)=7.91d-22*0.1*((es/eh)**2.5d0)*(eh/energ(j))**3
      end do
    end if
    do j=i,ndata
      eaus(j)=energ(j)
      iq=1
      ej=energ(j)-es
      call taylor(ndata,energ,ej,iq,x,y,z)
```

```

if (iq.eq.1) then
    faus=fdst(1)*y+fdst(2)*z
else if (iq.eq.ndata) then
    faus=fdst(ndata-1)*x+fdst(ndata)*y
else
    faus=fdst(iq-1)*x+fdst(iq)*y+fdst(iq+1)*z
end if
vaus(j)=qu(j)*faus*eaus(j)*eaus(j)
end do
call trapezi(ndata,eaus,vaus,1,ndata,r(ir))
r(ir)=r(ir)*(dsqrt(2.d0)/(cl*cl))*m**(-1.5d0)
r(ir)=r(ir)*g(ir)/(2*g(n_cr+1))
end do

return
end

```

**subroutine salvarisultati**

```

implicit none
integer i
include 'oggetti.fi'
include 'dati.fi'
include 'valori.fi'

open(unit=10,file='coeff.out',status='unknown')
do i=1,ndata
    write(10,99) i,energ(i)/e,K(i),U(i),gamma(i),dabs(dx(i))
end do
close (unit=10)
open(unit=10,file='a_funz.out',status='unknown')
do i=1,ndata
    write(10,98) energ(i)/e,A(i),DA(i)
end do
close (unit=10)

```

```

98      format (3g16.6)
99      format (i5,5g16.6)

```

```

end

```

**subroutine soluzione\_cr**

```
implicit none
include 'parametri_cr.fi'
integer ipath,i,j
parameter (ipath=1)

write(*,*)"Calcolo soluzione"

c      call dlslrg (n_cr,a_cr,n_cr,tn_cr,ipath,nk)
c      call dlsarg (n_cr,a_cr,n_cr,tn_cr,ipath,nk)

c      Calcolo flussi di popolazione percentuali

do i=2,n_cr
do j=1,n_cr
    fp(i,j)=-1.0d2*((a_cr(i,j)*nk(j))/(a_cr(i,i)*nk(i)))
end do
end do

c      Calcolo flusso

do j=1,n_cr
    s_cr=s_cr+sc_cr(j)*nk(j)
end do
fs=s_cr-alfa_cr

return
end
```

**subroutine soluzione**

```
implicit none
include 'oggetti.fi'
integer iparam(6),ipath,i
double precision rparam(5)
external dlslxg,dl4lxg

call dl4lxg(iparam,rparam)
```

```
ipath=1
iparam(5)=10000000

call dlslxg(ndata,nzero,AA,IA,JA,tn,ipath,iparam,rparam,fdst)

c      open (unit=10,file='fdist1.out',status='unknown')
c      do i=1,ndata
c          write(10,10) i,energ(i),fdst(i)
c      end do
c      close (10)

c10    format(i6,2g16.8)

      return
      end

subroutine taylor(nqu,x,ener,ie,a,b,c)

c      Subroutine che calcola i tre coefficienti A,B,C derivanti dalla approssimazione di
c      Taylor del      secondo ordine. Viene utilizzata per ogni funzione f generica
c      (sez d'urto, funzione di distribuzione...)
c      nqu: nr dei dati
c      x: vettore delle x
c      ener: valore di x al quale è richiesta la funzione
c      ie:      indice del punto più vicino (output)
c      a,b,c: i tre coefficienti di uscita

      implicit none
      integer nqu,i,ie,ix
      double precision ener,a,b,c,de,sx,dx,sum
      double precision x(nqu)

      a=0.d0
      b=0.d0
      c=0.d0
      ix=ie
      do i=ix,nqu
      if (ener.le.x(i)) then
          if (i.gt.1) then
              if((x(i)-ener).lt.(ener-x(i-1))) then
```

```

        ie=i
        else
            ie=i-1
        end if
        goto 5
    else
        ie=1
    end if
    goto 5
end if
end do
5   continue
if (ie.eq.1) then
    b=1.d0-(ener-x(ie))/(x(ie+1)-x(ie))
    c=(ener-x(ie))/(x(ie+1)-x(ie))
else if (ie.eq.nqu) then
    b=1.d0+(ener-x(ie-1))/(x(ie)-x(ie-1))
    a=-(ener-x(ie-1))/(x(ie)-x(ie-1))
else
    sx=x(ie)-x(ie-1)
    dx=x(ie+1)-x(ie)
    sum=dx+sx
    de=ener-x(ie)
    a=-(dx/(sx*sum))*de+(1.d0/(sx*sum))*de*de
    b=1.d0+(1.d0/sx-1.d0/dx)*de-(1.d0/(dx*sx))*de*de
    c=(sx/(dx*sum))*de+(1.d0/(dx*sum))*de*de
end if

return
end

```

### **subroutine temp**

```

implicit none
include 'dati.fi'
include 'oggetti.fi'
integer i
double precision faus(ndatamx)
include 'valori.fi'

```

```
Te=0.d0
do i=1,nidata
  faus(i)=energ(i)*dsqrt(energ(i))*fdst(i)
end do
call trapezi(nidata,energ,faus,1,nidata,Te)
Te=2.d0/3.d0*Te/kboltz

return
end

subroutine ter_ecc(necc,ndecc,qecc,ds,tecc,Iecc)

c      Questa subroutine genera le matrici terecc e Iecc.
c      Iecc: matrice degli indici di colonna dei punti traslati riferiti a be
c      tecc: matrice dei punti traslati ae,be,ce derivanti dall'approssimazione di Taylor
c            del 2° ordine.
c      ii rappresenta l'indice di eccitazione

implicit none
integer i,j,ii,icol,iq,necc
double precision caus,qu,x,y,z,ds,es,ae,be,ce
include 'dati.fi'
include 'oggetti.fi'
double precision tecc(ndatamx,3*necc),qecc(nqmax,2*necc)
integer IND(ndatamx),Iecc(ndatamx,necc),ndecc(necc)
include 'valori.fi'

c      Inizializzazione della matrice

do i=1,ndatamx
  do j=1,3*necc
    tecc(i,j)=0.d0
  end do
end do

do i=1,ndatamx
  do j=1,necc
    Iecc(i,j)=0
  end do
end do
```

```
do ii=1,necc
    do j=1,ndecc(ii)
        x0(j)=qecc(j,2*ii-1)
        f0(j)=qecc(j,2*ii)
    end do
    j=1
    iq=1
    do i=1,ndata
        es=energ(i)+qecc(1,2*ii-1)
        if (es.gt.enermax*e) then
            goto 10
        else
            call taylor(ndata,energ,es,j,x,y,z)
            Iecc(i,ii)=j
            ae=x
            be=y
            ce=z
            call taylor(ndecc(ii),x0,es,iq,x,y,z)
            if (iq.eq.1) then
                qu=f0(1)*y+f0(2)*z
            else if (iq.eq.ndecc(ii)) then
                qu=f0(ndecc(ii)-1)*x+f0(ndecc(ii))*y
            else
                qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z
            end if
            if (qu.lt.0.d0) then
                write(*,*) 'terecc.f',ii
            else
            end if
            icol=3*ii
            tec(i,icol-2)=ae*qu*es*ds*2.0/(k(i)*m*m)
            tec(i,icol-1)=be*qu*es*ds*2.0/(k(i)*m*m)
            tec(i,icol)=ce*qu*es*ds*2.0/(k(i)*m*m)
        end if
    end do
10     continue
    end do

    return
```

end

**subroutine ter\_ion(nion,ndion,qion,ds,eion,tion,Iion)**

c Questa subroutine genera le matrici terion e Iion.  
c Iion: matrice degli indici di colonna dei punti traslati riferiti a be  
c tion: matrice dei punti traslati ae,be,ce derivanti dall'approssimazione di Taylor  
c del 2° ordine.  
c Per ogni grado di ionizzazione nion ci sono 2 colonne relative alla ripartizione della  
c energia dopo l'urto.  
c ii rappresenta l'indice di ionizzazione  
c id rappresenta l'indice di ripartizione dell'energia dopo l'urto:  
c id=2\*ii-1 delta  
c id=2\*ii 1-delta

implicit none

integer i,j,ii,id,icol,iq,nion

double precision caus,qu,x,y,z,ds(nion),eion(nion)

double precision ae,be,ce,es

logical status

include 'dati.fi'

include 'oggetti.fi'

double precision tion(ndatamx,6\*nion),qion(nqmax,2\*nion)

integer IND(ndatamx),Iion(ndatamx,2\*nion),ndion(nion)

include 'valori.fi'

c Inizializzazione della matrice

do i=1,ndatamx

do j=1,6\*nion

tion(i,j)=0.d0

end do

end do

do i=1,ndatamx

do j=1,2\*nion

Iion(i,j)=0.d0

end do

end do

```
status=.true.

do ii=1,nion
  do j=1,ndion(ii)
    x0(j)=qion(j,2*ii-1)
    f0(j)=qion(j,2*ii)
  end do
20  if (status.eq..true.) then
      id=1
    else
      id=0
    end if
    iq=1
    j=1
  do i=1,ndata
    es=energ(i)/delta+eion(ii)
    if (es.gt.enermax*e) then
      goto 10
    else
      call taylor(ndata,energ,es,j,x,y,z)
      lion(i,ii)=j
      ae=x
      be=y
      ce=z
      call taylor(ndion(ii),x0,es,iq,x,y,z)
      if (iq.eq.1) then
        qu=f0(1)*y+f0(2)*z
      else if (iq.eq.ndion(ii)) then
        qu=f0(ndion(ii)-1)*x+f0(ndion(ii))*y
      else
        qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z
      end if
      if (qu.lt.0.d0) then
        write(*,*) 'terion.f',qu,ii
      else
      end if
      icol=3*(2*ii-id)
      tion(i,icol-2)=ae*qu*es*2.0*ds(ii)/(k(i)*delta*m*m)
      tion(i,icol-1)=be*qu*es*2.0*ds(ii)/(k(i)*delta*m*m)
      tion(i,icol)=ce*qu*es*2.0*ds(ii)/(k(i)*delta*m*m)
```

```
    end if
end do
10      continue
if (status.eq..true.) then
    status=.false.
    delta=1.d0-delta
    goto 20
else
    status=.true.
    delta=1.d0-delta
end if
continue
end do

return
end
```

**subroutine terminenoto**

```
implicit none
integer i,j,g
include 'dati.fi'
include 'oggetti.fi'
include 'valori.fi'

tn(1)=1.d0
do i=2,ndatamx
    tn(i)=0.d0
end do

return
end
```

**subroutine trapezi(nd,en,fa,imin,imax,integral)**

```
implicit none
double precision integral,mu
```

```
integer imin,imax,i,nd
double precision fa(nd),en(nd)

mu=0.d0
integral=0.d0
do i=imin+1,imax
  mu=(fa(i)+fa(i-1))*(en(i)-en(i-1))/2.d0
  integral=integral+mu
end do

return
end
```

**subroutine trovaa(iq,ener,aist,d)**

c Questa subroutine calcola il valore di A e della sua derivata in forma numerica

```
implicit none
integer i,iq
double precision aist,d,ener
double precision x,y,z,qu
double precision c1,c2,b0,sez,d1,d2,dsez(1),V(1)
include 'oggetti.fi'
double precision vaus(n_ionmax),daus(n_ionmax)
logical status
external dsplez
include 'dati.fi'
include 'dati_ar.fi'
include 'valori.fi'

aist=0.d0
d=0.d0
```

c Urti e-neutro

```
if (status.eq..false.) then
  do i=1,ndel_ar
    x0(i)=qel_ar(i,1)
    f0(i)=qel_ar(i,2)
    status=.true.
```

## APPENDIX B

---

```
end do  
else  
end if  
  
c      iq=1  
call taylor(ndel_ar,x0,ener,iq,x,y,z)  
if (iq.eq.1) then  
  qu=f0(1)*y+f0(2)*z  
else if (iq.eq.ndel_ar) then  
  qu=f0(ndel_ar-1)*x+f0(ndel_ar)*y  
else  
  qu=f0(iq-1)*x+f0(iq)*y+f0(iq+1)*z  
end if  
if (qu.lt.0.d0) then  
  write(*,*) 'MMMMMMMMMMMMMMMMMMMM'  
else  
end if  
vaus(1)=N_ar(1)*qu  
  
c      Derivata della sdu e-ArI  
  
V(1)=ener  
call dsplez(ndel_ar,x0,f0,1,1,1,V,dsez)  
daus(1)=N_ar(1)*dsez(1)  
  
c      Urto coulombiani e-ione  
  
ldebye=dsqrt(eps0*kboltz*Te/(Ne*e**2.d0))  
  
do i=2,nion_ar  
  
c      Calcolo dei contributi di A  
  
c1=i*(e**2.d0)/(8*Pi*eps0)  
b0=c1/ener  
c2=1+(ldebye/b0)**2.d0  
vaus(i)=dlog(dsqr(c2))  
vaus(i)=4*Pi*b0**2.d0*vaus(i)  
vaus(i)=N_ar(i)*vaus(i)
```

c       Calcolo della derivata analitica

```

d1=-b0**2*dlog(c2)
d2=(ldebye**2)/c2
daus(i)=4*Pi*(d1+d2)/ener
daus(i)=N_ar(i)*daus(i)

```

end do

c       Calcolo A(ener) e la sua derivata d(ener)

```

do i=1,nion_ar
aist=aist+vaus(i)
d=d+daus(i)
end do

```

c       Derivata di A in forma numerica

```

c DA(1)=(A(2)-A(1))/(ener(2)-ener(1))
c do i=2,ndata-1
c     denerdx=ener(i+1)-ener(i)
c     denersx=ener(i)-ener(i-1)
c     dener=denerdx+denersx
c     DA(i)=(A(i+1)-A(i))*denersx/(denerdx*dener)+
c 1     (A(i)-A(i-1))*denerdx/(denersx*dener)
c end do
c DA(ndata)=(A(ndata)-A(ndata-1))/(ener(ndata)-ener(ndata-1))

```

return

end

### **subroutine trovab**

```

implicit none
double precision c,gammaee
include 'dati.fi'
include 'oggetti.fi'
include 'valori.fi'

```

```
c=(12.d0*Pi*(eps0*kboltz*Te0)**(3.d0/2.d0))/(dsqrt(Ne)*e**3.d0)
```

```
gammaee=4.d0*Pi*((e**2.d0)/(4.d0*Pi*eps0*m))**2.d0*dlog(c)
```

```
B=gammaee*Ne
```

```
return
```

```
end
```

**subroutine udi(fa,ener,ien,aist,d,var,uist)**

```
implicit none
```

```
integer i,ien
```

```
double precision result3,result4
```

```
double precision dueterzi,ener,aist,d,uist
```

```
parameter (dueterzi=2.d0/3.d0)
```

```
double precision caus1,caus2,caus3,caus4,caus,uA
```

```
double precision vaus1,vaus2,vaus3,vaus4,vaus5,var
```

```
include 'oggetti.fi'
```

```
include 'dati.fi'
```

```
double precision fa(ndatamx)
```

```
include 'dati_ar.fi'
```

```
include 'valori.fi'
```

```
caus=e*campo/m
```

```
caus1=-dueterzi*caus*caus
```

```
caus2=(4.d0/3.d0)*(alfa*e*campo/(m*m))
```

```
caus3=4.d0/(m*m_ar)
```

```
caus4=kboltz*Th*caus3
```

```
uA=ener*aist
```

```
vaus1=caus1*((1.d0/aist)-(ener/(aist*aist))*d)
```

```
vaus2=caus2*ener/aist
```

```
vaus3=-caus3*ener*uA
```

```
vaus4=-caus4*(d*ener*ener+2.d0*uA)
```

c Contributo di Fokker-Plank

```
if (ien.eq.1) then
```

```
result4=0.d0
```

```
else
```

```
call trapezi(ndata0,energ0,fa,1,ien,result4)
```

```
end if
```

```
result3=dsqrt(energ0(ien))*var

vaus5=-B*(result3+result4)

c      Somma totale dei contributi

uist=vaus1+vaus2+vaus3+vaus4+vaus5

return
end

subroutine write_nk

implicit none
include 'parametri_cr.fi'
integer i,j

c      Stampa delle popolazioni

open (unit=10,file='n40_1.out',status='unknown')
write(10,*) fs
write(10,9) 'Livello [eV]','nk','n/g'
do i=1,n_cr+1
    write(10,10) elev(i),nk(i),dlog(nk(i)/g(i))
end do
close (10)

c      Stampa dei flussi

open (unit=10,file='fp40_1.out',status='unknown')
write(10,50) ((fp(i,j),j=1,n_cr),i=2,n_cr)
close (10)

9      format(a13,2a15)
10     format(3g16.8)
50     format(78e13.4)

return
end
```

**subroutine writeres**

```
implicit none
include 'oggetti.fi'
include 'dati.fi'
integer i
double precision maxw
external maxw
include 'dati_ar.fi'

open (unit=10,file='f40_1.out',status='unknown')
write(10,11) 'Temp. pesanti = ',Th, °K'
write(10,11) 'Campo elettrico = ',campo, 'V/m'
write(10,12) 'Densità = ',N, 'm-3'
write(10,13) 'Rapporto E/N = ',campo/N,'V*m^2',
1      ('campo*1.d21/N,'Td)'
write(10,11) 'Temperatura elettronica = ',Te, °K'
write(10,12) 'Velocità di drift = ',Vd,'m/s'
write(10,12) 'Freq. di ioniz. tot. = ',ni,'1/s'
write(10,12) 'Coeff. di ioniz. = ',alfa,'1/m'
write(10,12) 'alfa/Densità = ',alfa/N,'m^2'
write(10,12) 'N ArI = ',N_ar(1),'m^-3'
write(10,12) 'N ArII = ',N_ar(2),'m^-3'
write(10,12) 'N ArIII = ',N_ar(3),'m^-3'
write(10,9) 'Punto','Ener[J]','fdst','Maxwell','f/maxw','f1',
1           'f1/f0'
do i=1,ndata
  write(10,10) i,enereV(i),fdst(i),maxw(energ(i)),
1  fdst(i)/maxw(energ(i)),funo(i),dabs(funo(i)/fzero(i))
end do
close (10)

9   format(a6,5a14,a20)
10  format(i6,6g16.8)
11  format(a27,f7.0,a3)
12  format(a27,g10.3,a5)
13  format(a27,g10.3,a7,1x,a,f6.1,a4)

return
end
```

**subroutine zero**

```
implicit none
double precision maxw
external maxw
integer i
include 'oggetti.fi'

do i=1,ndata
  if ((fdst(i)).eq.(0.d0)) then
    goto 10
  else
    end if
    end do

10   write(*,*)"la funzione si annulla a',enereV(i),'elettronvolt'
      do i=1,ndata
        if ((fdst(i))/maxw(energ(i)).lt.1.d-10) then
          goto 20
        else
          end if
          end do

20   write(*,*)"la funzione si abbassa a',enereV(i),'elettronvolt'

      return
end
```

**dati.fi**

```
double precision m,e,Th,Te,Te0,Ne,eps0,Pi,kboltz,h,cl,
1           costmaxw,ldebye,b,enermax,delta,azero,Ryd,k1,
1           campo,alfa,N

common /dati/m,e,Th,Te,Te0,Ne,eps0,Pi,kboltz,h,cl,
1           costmaxw,ldebye,b,enermax,delta,azero,Ryd,k1,
1           campo,alfa,N
```

**dati\_ar.fi**

```
integer ndel_ar,nion_ar,necc1_ar1,necc1_ar2

double precision qion_ar(nqmax,2*n_ionmax)
double precision tion_ar(ndatamx,6*n_ionmax)
double precision qecc1_ar1(nqmax,2*n_eccmax)
double precision tecc1_ar1(ndatamx,3*n_eccmax)
double precision qecc1_ar2(nqmax,2*n_eccmax)
double precision tecc1_ar2(ndatamx,3*n_eccmax)
double precision n_ar(n_ionmax),eion_ar(n_ionmax)
double precision qel_ar(nqmax,2)
double precision m_ar

integer ndion_ar(n_ionmax)
integer Iion_ar(ndatamx,2*n_ionmax)
integer ndecc1_ar1(n_eccmax)
integer Iecc1_ar1(ndatamx,n_eccmax)
integer ndecc1_ar2(n_eccmax)
integer Iecc1_ar2(ndatamx,n_eccmax)

common /t_coll_ar/tion_ar,tecc1_ar1,tecc1_ar2
common /it_coll_ar/ion_ar,Iecc1_ar1,Iecc1_ar2
common /q_ar/qel_ar,qion_ar,qecc1_ar1,qecc1_ar2
common /nd_ar/ndel_ar,ndion_ar,ndecc1_ar1,ndecc1_ar2
common /nqdata_ar/nion_ar,necc1_ar1,necc1_ar2
common /dens_ar/n_ar,m_ar
common /stati_ar/eion_ar

eion_ar(1)=15.7596d0*e
eion_ar(2)=27.629d0*e
eion_ar(3)=40.74*e
m_ar=39.948*1.66d-27
```

**oggetti.fi**

```
integer ndatamx,n_ionmax,nqmax,n_eccmax,ndd
integer ndata,nzero,ndata0

parameter (ndatamx=10000,ndd=20)
parameter (nqmax=80,n_ionmax=3,n_eccmax=20)
```

```
double precision energ(ndatamx),energ0(ndatamx),
1          A(ndatamx),DA(ndatamx),K(ndatamx),parametro
double precision U(ndatamx),dx(ndatamx),gamma(ndatamx)
double precision AA(ndd*ndatamx),tn(ndatamx),integrale,nuovoalfa
double precision fdst(ndatamx),enereV(ndatamx),Vd,ni,Df(ndatamx),
1          dfzero(ndatamx),fzero(ndatamx),diffrel,conv,convint,
1          funo(ndatamx),fdst0(ndatamx),convtemp,convN
double precision x0(nqmax),f0(nqmax)

integer IA(ndd*ndatamx),JA(ndd*ndatamx),kr,itermax

common /crsectint/ndata,ndata0
common /crsectdp/energ,A,DA,enereV,energ0
common /risultati/K,U,dx,gamma,integrale,Vd,ni,nuovoalfa
common /mtx_dp/aa,fdst,tn,fzero,fdst0,diffrel,convN,
1          conv,convint,parametro,convtemp,dfzero,funo,Df
common /mtx_int/ia,ja,kr,itermax,nzero
```

**parametric\_cr.fi**

```
integer ntot_cr,n_cr
parameter (n_cr=78,ntot_cr=(n_cr+1)*(n_cr+1))

integer g(n_cr+1),l(n_cr+1)
double precision elev(n_cr+1),nk(n_cr+1)
double precision tn_cr(n_cr),fo(n_cr,n_cr),fp(n_cr,n_cr)
double precision a_cr(n_cr,n_cr),fs
double precision alfa_cr,s_cr,sc_cr(n_cr)

common /dati_liv/elev,g,l,tn_cr,fo
common /matrice_cr/a_cr,sc_cr
common /risultati_cr/nk,fp,fs,alfa_cr,s_cr
```

**valori.fi**

```
e=1.60217733d-19
eps0=8.854187817d-12
m=9.11e-31
h=6.626e-34
```

## APPENDIX B

---

```
kboltz=1.380658d-23
Pi=3.141592654
cl=2.998e8

enereV(1)=1.0d-3
enermax=1.0d2
parametro=2.0d-2

delta=0.5d0
alfa=0.d0

conv=5.0d-1
convtemp=1.d-4
convN=1.0d-3
itermax=1000

azero=0.529d-10
Ryd=13.6d0*e
k1=Pi*(2.d0*azero*Ryd)**2.d0
```