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14:22

Contents

1 genoei

Function to compute the one-electron integrals (overlap, kinetic energy and nuclear attraction). The STRUCTURES and GENOEI manual pages must be consulted for a detailed description of the calling sequence.

The overlap and kinetic energy integrals are expressed in terms of a basic one-dimensional Cartesian overlap component computed by **function** *ovrlap* while the more involved nuclear-attraction integrals are computed as a sum of geometrical factors computed by **subroutine** *aform* and the standard F_ν computed by **function** *fmch*.

"integral.f" 1 ≡
  @m *ERROR_OUTPUT_UNIT* 6

double precision function *genoei*(*i*, *j*, *eta*, *ngmx*, *nfirst*, *nlast*, *ntype*, *nr*, *ntmx*, *vlist*, *noc*, *ncmx*, *ovltot*, *kintot*) **implicit double precision** (*a* − *h*, *o* − *z*)
integer *i*, *j*, *ngmx*, *ncmx*, *noc*, *ntmx*
integer *nfirst*(∗), *nlast*(∗), *ntype*(∗), *nr*(*ntmx*, 3)
double precision *ovltot*, *kintot*
double precision *eta*(*MAX_PRIMITIVES*, 5), *vlist*(*MAX_CENTRES*, 4)

/∗ Insert delarations which are purely local to *genoei* ∗/

⟨ genoei local declarations 1.1 ⟩

/∗ Insert the Factorials ∗/

⟨ Factorials 4.2 ⟩

/∗ Obtain the powers of x,y,z and summation limits ∗/

⟨ One-electron Integer Setup 1.2 ⟩

/∗ Inter-nuclear distance ∗/

$rAB = (eta(iss,\ 1) - eta(jss,\ 1))^2 + (eta(iss,\ 2) - eta(jss,\ 2))^2 + (eta(iss,\ 3) - eta(jss,\ 3))^2$

/∗ Initialise all accumulators ∗/

genoei = *zero*
totnai = *zero*
kintot = *zero*
ovltot = *zero*

/∗ Now start the summations over the contracted GTFs ∗/

do *irun* = *iss*, *il* /∗ start of "i" contraction ∗/

  do *jrun* = *jss*, *jl* /∗ start of "j" contraction ∗/

    ⟨ Compute PA 4.4 ⟩ /∗ Use the Gaussian-product theorem to find $\vec{P}$ ∗/

    ⟨ Overlap Components 1.3 ⟩

    ovltot = *ovltot* + *anorm* ∗ *bnorm* ∗ *ovl* /∗ accumulate Overlap ∗/

    write (∗, ∗) *ovltot*, "HAPPY"

    ⟨ Kinetic Energy Components 2.1 ⟩

```
    kintot = kintot + anorm * bnorm * kin     /* accumulate Kinetic energy */
      /* now the nuclear attraction integral */
    tnai = zero
    ⟨ Form fj 2.2 ⟩     /* Generate the required f_j coefficients */
    do n = 1, noc     /* loop over nuclei */
      pn = zero     /* Initialise current contribution */
        /* Get the attracting-nucleus information; co-ordinates */
      ⟨ Nuclear data 3.1 ⟩
      t = t1 * pcsq
      call auxg(m, t, g)     /* Generate all the F_ν required */
      ⟨ Form As 2.3 ⟩     /* Generate the geometrical A-factors */
        /* Now sum the products of the geometrical A-factors and the F_ν */
      do ii = 1, imax
        do jj = 1, jmax
          do kk = 1, kmax
            nu = ii + jj + kk - 2
            pn = pn + Airu(ii) * Ajsv(jj) * Aktw(kk) * g(nu)
          end do
        end do
      end do
      tnai = tnai - pn * vn, 4 )     /* Add to total multiplied by currentrrent charge */
    end do     /* end of loop over nuclei */
    totnai = totnai + prefa * tnai
  end do     /* end of "j" contraction */
end do     /* end of "i" contraction */
genoei = totnai + kintot     /* "T + V" */
return end
```

These are the declarations which are local to *genoei*, working space *etc.*

```
⟨ genoei local declarations 1.1 ⟩ ≡
  double precision Airu(10), Ajsv(10), Aktw(10)
  double precision p(3), sf(10, 3), tf(20)
  double precision fact(20), g(50)
  double precision kin
  data zero, one, two, half, quart/0.0 · 10^00D, 1.0 · 10^00D, 2.0 · 10^00D, 0.5 · 10^00D, 0.25 · 10^00D/
  data pi/3.141592653589 · 10^00D/
```

This code is used in section 1.

Get the various powers of x, y and z required from the data structures and obtain the contraction limits etc.

⟨ One-electron Integer Setup 1.2 ⟩ ≡

```
ityp = ntype(i);
jtyp = ntype(j)
l1 = nr(ityp, 1);
m1 = nr(ityp, 2);
n1 = nr(ityp, 3)
l2 = nr(jtyp, 1);
m2 = nr(jtyp, 2);
n2 = nr(jtyp, 3)
imax = l1 + l2 + 1;
jmax = m1 + m2 + 1;
kmax = n1 + n2 + 1
maxall = imax
if (maxall < jmax)
  maxall = jmax
if (maxall < kmax)
  maxall = kmax
if (maxall < 2)
  maxall = 2    /* when all functions are "s" type */
iss = nfirst(i);
il = nlast(i)
jss = nfirst(j);
jl = nlast(j)
```

This code is used in section 1.

This simple code gets the Cartesian overlap components and assembles the total integral. It also computes the overlaps required to calculate the kinetic energy integral used in a later module.

⟨ Overlap Components 1.3 ⟩ ≡

```
prefa = two * prefa
expab = dexp(-aexp * bexp * rAB / t1)
s00 = (pi / t1)^1.5 * expab
dum = one;
tf(1) = one;
del = half / t1
do n = 2, maxall
  tf(n) = tf(n - 1) * dum * del
  dum = dum + two
end do

ox0 = ovrlap(l1, l2, pax, pbx, tf)
oy0 = ovrlap(m1, m2, pay, pby, tf)
oz0 = ovrlap(n1, n2, paz, pbz, tf)
ox2 = ovrlap(l1, l2 + 2, pax, pbx, tf)
oxm2 = ovrlap(l1, l2 - 2, pax, pbx, tf)
oy2 = ovrlap(m1, m2 + 2, pay, pby, tf)
oym2 = ovrlap(m1, m2 - 2, pay, pby, tf)
oz2 = ovrlap(n1, n2 + 2, paz, pbz, tf)
ozm2 = ovrlap(n1, n2 - 2, paz, pbz, tf)
ov0 = ox0 * oy0 * oz0;
ovl = ov0 * s00
ov1 = ox2 * oy0 * oz0;
ov4 = oxm2 * oy0 * oz0
ov2 = ox0 * oy2 * oz0;
ov5 = ox0 * oym2 * oz0
ov3 = ox0 * oy0 * oz2;
ov6 = ox0 * oy0 * ozm2
```

This code is used in section 1.

2 ovrlap

One-dimensional Cartesian overlap. This function uses the precomputed factors in *tf* to evaluate the simple Cartesian components of the overlap integral which must be multiplied together to form the total overlap integral.

"integral.f" 2 ≡

```
double precision function ovrlap(l1, l2, pax, pbx, tf)
  implicit double precision (a − h, o − z)
  integer l1, l2
  double precision pax, pbx
  double precision tf(∗)
      /∗ pre-computed exponent and double factorial factors: tf(i+1) = (2i-1)!/(2**i*(A+B)**i) ∗/
  double precision zero, one, dum
  data zero, one /0.0 · 10^00D, 1.0 · 10^00D/

  if ((l1 < 0) | (l2 < 0)) then
    ovrlap = zero
    return
  end if

  if ((l1 ≡ 0) ∧ (l2 ≡ 0)) then
    ovrlap = one
    return
  end if

  dum = zero;
  maxkk = (l1 + l2) / 2 + 1

  do kk = 1, maxkk
    dum = dum + tf(kk) ∗ fj(l1, l2, 2 ∗ kk − 2, pax, pbx)
  end do

  ovrlap = dum

  return
end
```

Use the previously-computed overlap components to generate the Kinetic energy components and hence the total integral.

⟨ Kinetic Energy Components 2.1 ⟩ ≡

```
xl = dfloat(l2 ∗ (l2 − 1));
xm = dfloat(m2 ∗ (m2 − 1))
xn = dfloat(n2 ∗ (n2 − 1));
xj = dfloat(2 ∗ (l2 + m2 + n2) + 3)
kin = s00 ∗ (bexp ∗ (xj ∗ ov0 − two ∗ bexp ∗ (ov1 + ov2 + ov3)) − half ∗ (xl ∗ ov4 + xm ∗ ov5 + xn ∗ ov6))
```

This code is used in section 1.

Form the f_j coefficients needed for the nuclear attraction integral.

```
⟨ Form fj 2.2 ⟩ ≡
    m = imax + jmax + kmax − 2
    do n = 1, imax
      sf(n, 1) = fj(l1, l2, n − 1, pax, pbx)
    end do

    do n = 1, jmax
      sf(n, 2) = fj(m1, m2, n − 1, pay, pby)
    end do

    do n = 1, kmax
      sf(n, 3) = fj(n1, n2, n − 1, paz, pbz)
    end do
```

This code is used in section 1.

Use *aform* to compute the required A-factors for each Cartesian component.

```
⟨ Form As 2.3 ⟩ ≡
    epsi = quart / t1
    do ii = 1, 10
      Airu(ii) = zero
      Ajsv(ii) = zero
      Aktw(ii) = zero
    end do

    call aform(imax, sf, fact, cpx, epsi, Airu, 1)    /* form A_{i,r,u} */
    call aform(jmax, sf, fact, cpy, epsi, Ajsv, 2)    /* form A_{j,s,v} */
    call aform(kmax, sf, fact, cpz, epsi, Aktw, 3)    /* form A_{k,t,w} */
```

This code is used in section 1.

3 aform

Compute the nuclear-attraction A factors. These quantitities arise from the components of the three position vectors of the two basis functions and the attracting centre with respect to the centre of the product Gaussian. There is one of these for each of the three dimensions of Cartesian space; a typical one (the x component) is:

$$A_{\ell,r,i}(\ell_1,\ell_2,\vec{A}_x,\vec{B}_x,\vec{C}_x,\gamma) = (-1)^\ell f_\ell(\ell_1,\ell_2,\vec{PA}_x,\vec{PB}_x)\frac{(-1)^i \ell!\vec{PC}_x^{\ell-2r-2i}\epsilon^{r+i}}{r!i!(\ell-2r-2i)!}$$

"integral.f" 3 ≡

```
subroutine aform(imax, sf, fact, cpx, epsi, Airu, xyorz)
  implicit double precision (a − h, o − z)
  integer imax, xyorz
  double precision Airu(∗), fact(∗), sf(10, ∗)
  double precision one
  data one/1.0 · 10^00D/
  do i = 1, imax
    ai = (−one)^(i−1) ∗ sf(i, xyorz) ∗ fact(i)
    irmax = (i − 1) / 2 + 1
    do ir = 1, irmax
      irumax = irmax − ir + 1
      do iru = 1, irumax
        iq = ir + iru − 2
        ip = i − 2 ∗ iq − 1
        at5 = one
        if (ip > 0)
          at5 = cpx^ip
        tiru = ai ∗ (−one)^(iru−1) ∗ at5 ∗ epsi^iq / (fact(ir) ∗ fact(iru) ∗ fact(ip + 1))
        nux = ip + iru
        Airu(nux) = Airu(nux) + tiru
      end do
    end do
  end do
  return
end
```

Get the co-ordinates of the attracting nucleus with respect to $\vec{P}$.

⟨ Nuclear data 3.1 ⟩ ≡

```
cpx = p(1) − vlist(n, 1)
cpy = p(2) − vlist(n, 2)
cpz = p(3) − vlist(n, 3)
pcsq = cpx ∗ cpx + cpy ∗ cpy + cpz ∗ cpz
```

This code is used in section 1.

4 generi

The general electron-repulsion integral formula for contracted Gaussian basis functions. The STRUCTURES and GENERI manual pages must be consulted for a detailed description of the calling sequence.

"integral.f" 4 ≡

double precision function *generi*(*i*, *j*, *k*, *l*, *xyorz*, *eta*, *ngmx*, *nfirst*, *nlast*, *ntype*, *nr*, *ntmx*)

implicit double precision (*a* − *h*, *o* − *z*)
integer *i*, *j*, *k*, *l*, *xyorz*, *ngmx*, *ntmx*
double precision *eta*(*MAX_PRIMITIVES*, 5)
integer *nfirst*(∗), *nlast*(∗), *ntype*(∗), *nr*(*ntmx*, 3)

/∗ Variables local to the function ∗/

⟨ generi local declarations 4.1 ⟩

/∗ Insert the **data** statement for the factorials ∗/

⟨ Factorials 4.2 ⟩

/∗ Get the various integers from the data structures for the summation limits, Cartesian monomial powers etc. from the main integer data structures ∗/

⟨ Two-electron Integer Setup 4.3 ⟩

/∗ Two internuclear distances this time ∗/

$rAB = (eta(is,\ 1) - eta(js,\ 1))^2 + (eta(is,\ 2) - eta(js,\ 2))^2 + (eta(is,\ 3) - eta(js,\ 3))^2$
$rCD = (eta(ks,\ 1) - eta(ls,\ 1))^2 + (eta(ks,\ 2) - eta(ls,\ 2))^2 + (eta(ks,\ 3) - eta(ls,\ 3))^2$

/∗ Initialise the accumulator ∗/

generi = *zero*

/∗ Now the real work, begin the four contraction loops ∗/

do *irun* = *is*, *il* /∗ start of "i" contraction ∗/

do *jrun* = *js*, *jl* /∗ start of "j" contraction ∗/

/∗ Get the data for the two basis functions referring to electron 1; orbital exponents and Cartesian co-ordinates and hence compute the vector $\vec{P}$ and the components of $\vec{PA}$ and $\vec{PB}$ ∗/

⟨ Compute PA 4.4 ⟩

/∗ Use **function** *fj* and **subroutine** *theta* to calculate the geometric factors arising from the expansion of the product of Cartesian monomials for the basis functions of electron 1 ∗/

⟨ Thetas for electron 1 4.6 ⟩

do *krun* = *ks*, *kl* /∗ start of "k" contraction ∗/
do *lrun* = *ls*, *ll* /∗ start of "l" contraction ∗/
eribit = *zero* /∗ local accumulator ∗/

/∗ Get the data for the two basis functions referring to electron 2; orbital exponents and Cartesian co-ordinates and hence compute the vector $\vec{Q}$ and the components of $\vec{QC}$ and $\vec{QD}$ ∗/

⟨ Compute QC 4.5 ⟩

```
    w = pi / (t1 + t2)

      /* Repeat the use of function fj to obtain the geometric factors arising from the
        expansion of Cartesian monomials for the basis functions of electron 2 */

    ⟨ fj for electron 2 4.7 ⟩

    call auxg(m, t, g)    /* Obtain the F_ν by recursion */

      /* Now use the pre-computed θ factors for both electron distributions to form the overall
        B factors */

    ⟨ Form Bs 4.8 ⟩

      /* Form the limits and add up all the bits, the products of x, y and z related B factors
        and the F_ν */

    jt1 = i1max + i2max − 1
    jt2 = j1max + j2max − 1
    jt3 = k1max + k2max − 1

    do ii = 1, jt1
      do jj = 1, jt2
        do kk = 1, jt3
          nu = ii + jj + kk − 2
          if (xyorz ≠ 0)
            nu = nu + 1

            /* eribit is a repulsion integral over primitive GTFs */

          eribit = eribit + g(nu) * bbx(ii) * bby(jj) * bbz(kk)

        end do
      end do
    end do

      /* Now accumulate the primitive integrals into the integral over contracted GTFs
        including some constant factors and contraction coefficients */

    generi = generi + prefa * prefc * eribit * dsqrt(w)

  end do    /* end of "l" contraction loop */
 end do    /* end of "k" contraction loop */
end do    /* end of "j" contraction loop */
end do    /* end of "i" contraction loop */

if (xyorz ≡ 0)
  generi = generi * two
return
end
```

Here are the local declarations (workspoace *etc.*) for the two-electron main function *generi*.

⟨ generi local declarations 4.1 ⟩ ≡
```
double precision p(3), q(3), ppx(20), ppy(20), ppz(20)
double precision bbx(20), bby(20), bbz(20), sf(10, 6)
double precision xleft(5, 10), yleft(5, 10), zleft(5, 10)
double precision r(3), fact(20), g(50)
data zero, one, two, half /0.0 · 10^00D, 1.0 · 10^00D, 2.0 · 10^00D, 0.5 · 10^00D/
data pi/3.141592653589 · 10^00D/
```

This code is used in section 4.

These numbers are the first 20 factorials $fact(i)$ contains $(i-1)!$.

⟨ Factorials 4.2 ⟩ ≡
```
data fact/1.0 · 10^00D, 1.0 · 10^00D, 2.0 · 10^00D, 6.0 · 10^00D, 24.0 · 10^00D, 120.0 · 10^00D, 720.0 · 10^00D,
    5040.0 · 10^00D, 40320.0 · 10^00D, 362880.0 · 10^00D, 3628800.0 · 10^00D, 39916800.0 · 10^00D,
    479001600.0 · 10^00D, 6227020800.0 · 10^00D, 6 ∗ 0.0 · 10^00D/
```

This code is used in sections 1, 4, and 5.

This tedious code extracts the (integer) setup data; the powers of x, y and z in each of the Cartesian monomials of each of the four basis functions and the limits of the contraction in each case.

⟨ Two-electron Integer Setup 4.3 ⟩ ≡
```
ityp = ntype(i)
jtyp = ntype(j)
ktyp = ntype(k)
ltyp = ntype(l)
l1 = nr(ityp, 1)
m1 = nr(ityp, 2)
n1 = nr(ityp, 3)
l2 = nr(jtyp, 1)
m2 = nr(jtyp, 2)
n2 = nr(jtyp, 3)
l3 = nr(ktyp, 1)
m3 = nr(ktyp, 2)
n3 = nr(ktyp, 3)
l4 = nr(ltyp, 1)
m4 = nr(ltyp, 2)
n4 = nr(ltyp, 3)
is = nfirst(i)
il = nlast(i)
js = nfirst(j)
jl = nlast(j)
ks = nfirst(k)
kl = nlast(k)
ls = nfirst(l)
ll = nlast(l)
```

This code is used in section 4.

Use the Gaussian Product Theorem to find the position vector $\vec{P}$, of the product of the two Gaussian exponential factors of the basis functions for electron 1.

⟨ Compute PA 4.4 ⟩ ≡

```
aexp = eta(irun, 4);
anorm = eta(irun, 5)
bexp = eta(jrun, 4);
bnorm = eta(jrun, 5)

  /* aexp and bexp are the primitive GTF exponents for GTF irun and jrun, anorm and bnorm are
     the corresponding contraction coefficients bundled up into prefa */

t1 = aexp + bexp;
deleft = one / t1

p(1) = (aexp * eta(irun, 1) + bexp * eta(jrun, 1)) * deleft
p(2) = (aexp * eta(irun, 2) + bexp * eta(jrun, 2)) * deleft
p(3) = (aexp * eta(irun, 3) + bexp * eta(jrun, 3)) * deleft

pax = p(1) - eta(irun, 1)
pay = p(2) - eta(irun, 2)
paz = p(3) - eta(irun, 3)

pbx = p(1) - eta(jrun, 1)
pby = p(2) - eta(jrun, 2)
pbz = p(3) - eta(jrun, 3)

prefa = dexp(-aexp * bexp * rAB / t1) * pi * anorm * bnorm / t1
```

This code is used in sections 1 and 4.

Use the Gaussian Product Theorem to find the position vector $\vec{Q}$, of the product of the two Gaussian exponential factors of the basis functions for electron 2.

⟨ Compute QC 4.5 ⟩ ≡

```
cexpp = eta(krun, 4);
cnorm = eta(krun, 5)
dexpp = eta(lrun, 4);
dnorm = eta(lrun, 5)

  /* cexp and dexp are the primitive GTF exponents for GTF krun and lrun, cnorm and dnorm are
     the corresponding contraction coefficients bundled up into prefc */

t2 = cexpp + dexpp
t2m1 = one / t2
fordel = t2m1 + deleft

q(1) = (cexpp * eta(krun, 1) + dexpp * eta(lrun, 1)) * t2m1
q(2) = (cexpp * eta(krun, 2) + dexpp * eta(lrun, 2)) * t2m1
q(3) = (cexpp * eta(krun, 3) + dexpp * eta(lrun, 3)) * t2m1

qcx = q(1) - eta(krun, 1)
qcy = q(2) - eta(krun, 2)
qcz = q(3) - eta(krun, 3)

qdx = q(1) - eta(lrun, 1)
qdy = q(2) - eta(lrun, 2)
qdz = q(3) - eta(lrun, 3)

r(1) = p(1) - q(1)
r(2) = p(2) - q(2)
r(3) = p(3) - q(3)

t = (r(1) * r(1) + r(2) * r(2) + r(3) * r(3)) / fordel
prefc = exp(-cexpp * dexpp * rCD / t2 ) * pi * cnorm * dnorm / t2
```

This code is used in section 4.

The series of terms arising from the expansion of the Cartesian monomials like $(x - PA)^{\ell_1}(x - PB)^{\ell_2}$ are computed by first forming the f_j and hence the θs.

```
⟨ Thetas for electron 1 4.6 ⟩ ≡
    i1max = l1 + l2 + 1
    j1max = m1 + m2 + 1
    k1max = n1 + n2 + 1

    mleft = i1max + j1max + k1max

    do n = 1, i1max
      sf(n, 1) = fj(l1, l2, n − 1, pax, pbx)
    end do

    do n = 1, j1max
      sf(n, 2) = fj(m1, m2, n − 1, pay, pby)
    end do

    do n = 1, k1max
      sf(n, 3) = fj(n1, n2, n − 1, paz, pbz)
    end do

    call theta(i1max, sf, 1, fact, t1, xleft)
    call theta(j1max, sf, 2, fact, t1, yleft)
    call theta(k1max, sf, 3, fact, t1, zleft)
```

This code is used in section 4.

The series of terms arising from the expansion of the Cartesian monomials like $(x - QC)^{\ell_3}(x - QD)^{\ell_4}$ are computed by forming the f_j and storing them in the array *sf* for later use by *bform*.

```
⟨ fj for electron 2 4.7 ⟩ ≡
    i2max = l3 + l4 + 1
    j2max = m3 + m4 + 1
    k2max = n3 + n4 + 1

    twodel = half ∗ fordel
    delta = half ∗ twodel

    do n = 1, i2max
      sf(n, 4) = fj(l3, l4, n − 1, qcx, qdx)
    end do

    do n = 1, j2max
      sf(n, 5) = fj(m3, m4, n − 1, qcy, qdy)
    end do

    do n = 1, k2max
      sf(n, 6) = fj(n3, n4, n − 1, qcz, qdz)
    end do

    m = mleft + i2max + j2max + k2max + 1
```

This code is used in section 4.

In the central inner loops of the four contractions, use the previously- computed θ factors to form the combined geometrical B factors.

⟨ Form Bs 4.8 ⟩ ≡

```
ppx(1) = one;
bbx(1) = zero
ppy(1) = one;
bby(1) = zero
ppz(1) = one;
bbz(1) = zero

jt1 = i1max + i2max
do n = 2, jt1
  ppx(n) = -ppx(n-1) * r(1)
  bbx(n) = zero
end do

jt1 = j1max + j2max
do n = 2, jt1
  ppy(n) = -ppy(n-1) * r(2)
  bby(n) = zero
end do

jt1 = k1max + k2max
do n = 2, jt1
  ppz(n) = -ppz(n-1) * r(3)
  bbz(n) = zero
end do

call bform(i1max, i2max, sf, 1, fact, xleft, t2, delta, ppx, bbx, xyorz)
call bform(j1max, j2max, sf, 2, fact, yleft, t2, delta, ppy, bby, xyorz)
call bform(k1max, k2max, sf, 3, fact, zleft, t2, delta, ppz, bbz, xyorz)
```

This code is used in section 4.

5 fj

This is the function to evaluate the coefficient of x^j in the expansion of

$$(x+a)^\ell (x+b)^m$$

The full expression is

$$f_j(\ell, m, a, b) = \sum_{k=max(0,j-m)}^{min(j,\ell} \binom{\ell}{k}\binom{m}{j-k} a^{\ell-k} b^{m+k-j}$$

The function must take steps to do the right thing for 0.0^0 when it occurs.

"integral.f" 5 ≡

```
double precision function fj(l, m, j, a, b)
  implicit double precision (a − h, o − z)
  integer l, m, j
  double precision a, b
  double precision sum, term, aa, bb
  integer i, imax, imin
  double precision fact(20)
  ⟨ Factorials 4.2 ⟩
  imax = min(j, l)
  imin = max(0, j − m)
  sum = 0.0 · 10^00D
  do i = imin, imax
    term = fact(l + 1) ∗ fact(m + 1) / (fact(i + 1) ∗ fact(j − i + 1))
    term = term / (fact(l − i + 1) ∗ fact(m − j + i + 1))
    aa = 1.0 · 10^00D;
    bb = 1.0 · 10^00D
    if ((l − i) ≠ 0)
      aa = a^(l−i)
    if ((m + i − j) ≠ 0)
      bb = b^(m+i−j)
    term = term ∗ aa ∗ bb
    sum = sum + term
  end do
  fj = sum
  return
end
```

6 theta

Computation of all the θ factors required from one basis-function product; any one of them is given by

$$\theta(j,\ell_1,\ell_2,a,b,r,\gamma) = f_j(\ell_1,\ell_2,a,b)\frac{j!\gamma^{r-j}}{r!(j-2r)!}$$

The f_j are computed in the body of *generi* and passed to this routine in *sf*, the particular ones to use are in *sf*(∗, *isf*). They are stored in *xleft*, *yleft* and *zleft* because they are associated with electron 1 (the left-hand factor in the integrand as it is usually written $(ij,k\ell)$).

"integral.f" 6 ≡

```
subroutine theta(i1max, sf, isf, fact, t1, xleft)
  implicit double precision (a − h, o − z)
  integer i1max, isf
  double precision t1
  double precision sf(10, ∗), fact(∗), xleft(5, ∗)
  integer i1, ir1, ir1max, jt2
  double precision zero, sfab, bbb
  data zero/0.0 · 10^00D/
  do i1 = 1, 10
    do ir1 = 1, 5
      xleft(ir1, i1) = zero
    end do
  end do
  do 100 i1 = 1, i1max
    sfab = sf(i1, isf)
    if (sfab ≡ zero)
      go to 100
    ir1max = (i1 − 1) / 2 + 1
    bbb = sfab ∗ fact(i1) / t1^(i1−1)
    do ir1 = 1, ir1max
      jt2 = i1 + 2 − ir1 − ir1
      xleft(ir1, i1) = bbb ∗ (t1^(ir1−1)) / (fact(ir1) ∗ fact(jt2))
    end do
100: continue
  return
end
```

7 bform

Use the pre-computed f_j and θ to form the "B " factors, the final geometrical expansion coefficients arising from the products of Cartesian monomials. Any one of them is given by

$$\begin{aligned} & B_{\ell,\ell',r_1,r_2,i}(\ell_1,\ell_2,\vec{A}_x,\vec{B}_x,\vec{P}_x,\gamma_1;\ell_3,\ell_4,\vec{C}_x,\vec{D}_x,\vec{Q}_x,\gamma_2) \\ = (-1)^{\ell'}\theta(\ell,\ell_1,\ell_2,\vec{PA}_x,\vec{PB}_x,r,\gamma_1)\theta(\ell',\ell_3,\ell_4,\vec{QC}_x,\vec{QD}_x,r',\gamma_2) \\ \times\frac{(-1)^i(2\delta)^{2(r+r')}(\ell+\ell'-2r-2r')!\delta^i\vec{p}_x^{\,\ell+\ell'-2(r+r'+i)}}{(4\delta)^{\ell+\ell'}i![\ell+\ell'-2(r+r'+i)]!} \end{aligned}$$

"integral.f" 7 ≡

```
subroutine bform(i1max, i2max, sf, isf, fact, xleft, t2, delta, ppx, bbx, xyorz)
  implicit double precision (a − h, o − z)
  integer i1max, i2max, isf
  double precision fact(∗), sf(10, ∗), xleft(5, ∗), bbx(∗), ppx(20)
  double precision delta
  integer xyorz, itab
  double precision zero, one, two, twodel, fordel, sfab, sfcd
  double precision bbc, bbd, bbe, bbf, bbg, ppqq
  integer i1, i2, jt1, jt2, ir1max, ir2max
  data zero, one, two/0.0 · 10^00D, 1.0 · 10^00D, 2.0 · 10^00D/
  itab = 0
  if (xyorz ≡ isf)
    itab = 1
  twodel = two ∗ delta;
  fordel = two ∗ twodel
  do 200 i1 = 1, i1max
    sfab = sf(i1, isf)
    if (sfab ≡ zero)
      go to 200
    ir1max = (i1 − 1) / 2 + 1
    do 210 i2 = 1, i2max
      sfcd = sf(i2, isf + 3)
      if (sfcd ≡ zero)
        go to 210
      jt1 = i1 + i2 − 2
      ir2max = (i2 − 1) / 2 + 1
      bbc = ((−one)^(i2−1)) ∗ sfcd ∗ fact(i2) / (t2^(i2−1) ∗ (fordel^jt1))
      do 220 ir1 = 1, ir1max
        jt2 = i1 + 2 − ir1 − ir1
        bbd = bbc ∗ xleft(ir1, i1)
        if (bbd ≡ zero)
          go to 220
```

```
      do 230 ir2 = 1, ir2max
        jt3 = i2 + 2 - ir2 - ir2
        jt4 = jt2 + jt3 - 2
        irumax = (jt4 + itab) / 2 + 1
        jt1 = ir1 + ir1 + ir2 + ir2 - 4
        bbe = bbd * (t2**(ir2-1)) * (twodel**jt1) * fact(jt4 + 1) / (fact(ir2) * fact(jt3))
        do 240 iru = 1, irumax
          jt5 = jt4 - iru - iru + 3
          ppqq = ppx(jt5)
          if (ppqq .eq. zero)
            go to 240
          bbf = bbe * ((-delta)**(iru-1)) * ppqq / (fact(iru) * fact(jt5))
          bbg = one
          if (itab .eq. 1) then
            bbg = dfloat(jt4 + 1) * ppx(2) / (delta * dfloat(jt5))
          end if
          bbf = bbf * bbg
          nux = jt4 - iru + 2
          bbx(nux) = bbx(nux) + bbf
  240   continue
  230 continue
  220 continue
  210 continue
  200 continue

      return
      end
```

8 auxg

Find the maximum value of F_ν required, use *fmch* to compute it and obtain all the lower F_ν by downward recursion.

$$F_{\nu-1}(x) = \frac{\exp(-x) + 2xF_\nu(x)}{2\nu - 1}$$

"integral.f" 8 ≡

```
subroutine auxg(mmax, x, g)
  implicit double precision (a − h, o − z)
  integer mmax
  double precision x, g(∗)
  double precision fmch
  double precision two, y
  integer mp1mx, mp1, md, mdm
  data two/2.0 · 10^00D/
  y = dexp(−x)
  mp1mx = mmax + 1
  g(mp1mx) = fmch(mmax, x, y)
  if (mmax < 1)
    go to 303    /∗ just in case! ∗/
  /∗ Now do the recursion downwards ∗/
  do mp1 = 1, mmax
    md = mp1mx − mp1
    mdm = md − 1
    g(md) = (two ∗ x ∗ g(md + 1) + y) / dfloat(2 ∗ mdm + 1)
  end do
303: return
  end
```

9 fmch

This code is for the oldest and most general and reliable of the methods of computing

$$F_\nu(x) = \int_0^1 t^{2\nu} \exp(-xt^2) dt \tag{1}$$

One of two possible series expansions is used depending on the value of x.

For $x \leq 10$ (Small x Case) the (potentially) infinite series

$$F_\nu(x) = \frac{1}{2} \exp(-x) \sum_{i=0}^{\infty} \frac{\Gamma(\nu + \frac{1}{2})}{\Gamma(\nu + i + \frac{3}{2})} x^i \tag{2}$$

is used.

The series is truncated when the value of terms falls below 10^{-8}. However, if the series seems to be becoming unreasonably long before this condition is reached (more than 50 terms), the evaluation is stopped and the function aborted with an error message on *ERROR_OUTPUT_UNIT*.

If $x > 10$ (Large x Case) a different series expansion is used:

$$F_\nu(x) = \frac{\Gamma(\nu + \frac{1}{2})}{2x^{\nu+\frac{1}{2}}} - \frac{1}{2} \exp(-x) \sum_{i=0}^{\infty} \frac{\Gamma(\nu + \frac{1}{2})}{\Gamma(\nu - i + \frac{3}{2})} x^{-i} \tag{3}$$

This series, in fact, diverges but it diverges so slowly that the error obtained in truncating it is always less than the last term in the truncated series. Thus, Thus, to obtain a value of the function to the same accuracy as the other series, the expansion is terminated when the last term is less than the same criterion (10^{-8}).

It can be shown that the minimum term is always for i close to $\nu + x$, thus ifthe terms for this value of i are not below the criterion, the series expansion is abandoned, a message output on *ERROR_OUTPUT_UNIT* and the function aborted.

The third argument, y, is $exp(-x)$, since it is assumed that this function will only be used *once* to evaluate the function $F_\nu(x)$ for the maximum value of ν required and other values will be obtained by downward recursion of the form

$$F_{\nu-1}(x) = \frac{\exp(-x) + 2xF_\nu(x)}{2\nu - 1} \tag{4}$$

which also requires the value of $\exp(-x)$ to be available.

NAME

fmch

SYNOPSIS

```
double precision function fmch(nu,x,y)

implicit double precision (a-h,o-z)
double precision x, y
integer nu
```

DESCRIPTION

Computes

$$F_\nu(x) = \int_0^1 t^{2\nu} e^{-xt^2} dt$$

given ν and x. It is used in the evaluation of GTF nuclear attraction and electron-repulsion integrals.

ARGUMENTS

nu Input: The value of ν in the explicit formula above (`integer`)

x Input: x in the formula (`double precision`)

y Input: $\exp(-x)$, assumed to be available.

DIAGNOSTICS

If the relevant series of expansion used do not converge to a tolerance of 10^{-8}, an error message is printed on standard output and the computation aborted.

"integral.f" 9 ≡

double precision function *fmch*(*nu*, *x*, *y*)
⟨ Declarations 9.1 ⟩ /∗ First, make the variable declarations ∗/
⟨ Internal Declarations 9.2 ⟩
m = *nu*
a = ***dfloat***(*m*)
if (*x* ≤ *ten*) **then**
⟨ Small x Case 9.3 ⟩
else
⟨ Large x Case 9.4 ⟩
end if
end

Here are the declarations and **data** statements which are ...

⟨ Declarations 9.1 ⟩ ≡

```
implicit double precision (a − h, o − z)
double precision x, y
integer nu
```

This code is used in section 9.

⟨ Internal Declarations 9.2 ⟩ ≡

```
double precision ten, half, one, zero, rootpi4, xd, crit
double precision term, partialsum
integer m, i, numberofterms, maxone, maxtwo
data zero, half, one, rootpi4, ten/0.0 · 10^00D, 0.5 · 10^00D, 1.0 · 10^00D, 0.88622692 · 10^00D, 10.0 · 10^00D/
    /* crit is required accuracy of the series expansion */
data crit/1.0 · 10^−08D/    /* maxone */
data maxone/50/, maxtwo/200/
```

This code is used in section 9.

⟨ Small x Case 9.3 ⟩ ≡

```
a = a + half
term = one / a
partialsum = term
do i = 2, maxone
  a = a + one
  term = term * x / a
  partialsum = partialsum + term
  if (term / partialsum < crit)
    go to 111
end do
111: continue
  if (i ≡ maxone) then
    write (ERROR_OUTPUT_UNIT, 200)
  200: format ('i␣>␣50␣in␣fmch')
    STOP
  end if
  fmch = half * partialsum * y
  return
```

This code is used in section 9.

```
⟨ Large x Case 9.4 ⟩ ≡
    b = a + half
    a = a − half
    xd = one / x
    approx = rootpi4 ∗ dsqrt(xd) ∗ xd^m
    if (m > 0) then
      do i = 1, m
        b = b − one
        approx = approx ∗ b
      end do
    end if
    fimult = half ∗ y ∗ xd
    partialsum = zero

    if (fimult ≡ zero) then
      fmch = approx
      return
    end if

    fiprop = fimult / approx
    term = one
    partialsum = term
    numberofterms = maxtwo
    do i = 2, numberofterms
      term = term ∗ a ∗ xd
      partialsum = partialsum + term
      if (dabs(term ∗ fiprop / partialsum) ≤ crit) then
        fmch = approx − fimult ∗ partialsum
        return
      end if
      a = a − one
    end do
    write(ERROR_OUTPUT_UNIT, 201)
201: format('␣numberofterms␣reached␣in␣fmch')
    STOP
```

This code is used in section 9.

10 INDEX

⟨ Compute PA 4.4 ⟩ Used in sections 1 and 4.
⟨ Compute QC 4.5 ⟩ Used in section 4.
⟨ Declarations 9.1 ⟩ Used in section 9.
⟨ Factorials 4.2 ⟩ Used in sections 1, 4, and 5.
⟨ Form As 2.3 ⟩ Used in section 1.
⟨ Form Bs 4.8 ⟩ Used in section 4.
⟨ Form fj 2.2 ⟩ Used in section 1.
⟨ Internal Declarations 9.2 ⟩ Used in section 9.
⟨ Kinetic Energy Components 2.1 ⟩ Used in section 1.
⟨ Large x Case 9.4 ⟩ Used in section 9.
⟨ Nuclear data 3.1 ⟩ Used in section 1.
⟨ One-electron Integer Setup 1.2 ⟩ Used in section 1.
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⟨ Thetas for electron 1 4.6 ⟩ Used in section 4.
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⟨ generi local declarations 4.1 ⟩ Used in section 4.
⟨ genoei local declarations 1.1 ⟩ Used in section 1.

COMMAND LINE: `"fweave integral.web"`.
WEB FILE: `"integral.web"`.
CHANGE FILE: `(none)`.
GLOBAL LANGUAGE: FORTRAN.