

```

! Loop on all k-points : num_kpoints = (2*n_max+1)*(2*l_max*m_max+l_max+m_max)
do imode = 1, num_kpoints
! Setup the current k-point (l,m,n) triplet
call compute_kmode_index(imode, l, m, n)

! cos_ky/sin_ky are stored only for m>= 0
mabs = abs(m)
sign_m = real(sign(1,m), wp)

! cos_kz/sin_kz are stored only for n>= 0
nabs = abs(n)
sign_n = real(sign(1,n), wp)

! Compute the norm squared of the k-point
kx = real(l,wp) * twopi / a
ky = real(m,wp) * twopi / b
kz = real(n,wp) * twopi / c
knorm2 = kx*kx + ky*ky + kz*kz

if (knorm2 <= knorm2_max) then

! Compute Sk_cos/Sk_sin for this (l,m,n) k-point
Sk_cos = 0.0_wp
Sk_sin = 0.0_wp
do j = 1, num_atoms
! load precomputed cos/sin values
cos_kx = cos_kx_elec(j,l)
sin_kx = sin_kx_elec(j,l)
cos_ky = cos_ky_elec(j,mabs)
sin_ky = sin_ky_elec(j,mabs) * sign_m
cos_kz = cos_kz_elec(j,nabs)
sin_kz = sin_kz_elec(j,nabs) * sign_n

! Compute cos/sin values using trigonometric rules
cos_kxky = cos_kx * cos_ky - sin_kx * sin_ky
sin_kxky = sin_kx * cos_ky + cos_kx * sin_ky
cos_kxkykz = cos_kxky * cos_kz - sin_kxky * sin_kz
sin_kxkykz = sin_kxky * cos_kz + cos_kxky * sin_kz

Sk_cos = Sk_cos + q_elec(j)*cos_kxkykz
Sk_sin = Sk_sin + q_elec(j)*sin_kxkykz
end do

! For each atom, compute the contribution of this k-point to the potential
Sk_alpha = 2.0_wp * (4.0_wp*pi/(a*b*c)) * exp(-knorm2/(4*alphasq))/knorm2
do i = 1, num_atoms
! Load precomputed cos/sin values
cos_kx = cos_kx_elec(i,l)
sin_kx = sin_kx_elec(i,l)
cos_ky = cos_ky_elec(i,mabs)
sin_ky = sin_ky_elec(i,mabs) * sign_m
cos_kz = cos_kz_elec(i,nabs)
sin_kz = sin_kz_elec(i,nabs) * sign_n

! Compute cos/sin values using trigonometric rules
cos_kxky = cos_kx * cos_ky - sin_kx * sin_ky
sin_kxky = sin_kx * cos_ky + cos_kx * sin_ky
cos_kxkykz = cos_kxky * cos_kz - sin_kxky * sin_kz
sin_kxkykz = sin_kxky * cos_kz + cos_kxky * sin_kz

V(i) = V(i) + Sk_alpha * (Sk_cos * cos_kxkykz + Sk_sin * sin_kxkykz)
end do
end if
end do

```