

```
Sk_cos(:) = 0.0_wp
Sk_sin(:) = 0.0_wp
```

```
num_blocks = (num_atoms-1) / block_vector_size + 1
```

```
! Compute Sk_cos/Sk_sin for each k-point
do iblock = 1, num_blocks
  (...)
  ! Loop on local k-points
  do imode = imode_start, imode_end
    (...)
    if (knorm2 <= knorm2_max) then
      ! Compute block contribution to Sk_cos/Sk_sin for this (l,m,n) k-point
      do j = jstart_block, jend_block
        (...)
        Sk_cos(imode) = Sk_cos(imode) + q_elec(j)*cos_kxkykz
        Sk_sin(imode) = Sk_sin(imode) + q_elec(j)*sin_kxkykz
      end do
    end if
  end do
end do
```

```
! Compute potential on each electrode atom
do iblock = 1, num_blocks
  (...)
  ! Loop on local k-points
  do imode = imode_start, imode_end
    (...)
    if (knorm2 <= knorm2_max) then
      ! For each atom, compute the contribution of this k-point to the potential
      (...)
      do i = istart_block, iend_block
        (...)
        V_local(i) = V_local(i) + Sk_alpha * (Sk_cos(imode)*cos_kxkykz &
          + Sk_sin(imode)*sin_kxkykz)
      end do
    end if
  end do
end do
```

```
call MPI_allreduce(V_local(:),V_global(:), num_atoms, &
  MPI_DOUBLE_PRECISION, MPI_SUM, MPI_COMM_WORLD, ierr)
```