

```

! Compute contribution from blocks on the diagonal
do iblock = 1, num_block_diag
  call compute_diag_block_boundaries(iblock, istart, iend)
  do i = istart, iend
    do j = istart, iend
      zij = z(j) - z(i)
      zijsq = zij * zij
      pot_ij = volfactor * (sqrpialpha * exp(-zijsq*alphasq) &
                            + pi * zij * erf(zij*alpha))
      V(i) = V(i) - q_elec(j) * pot_ij
    end do
  end do
end do

! Compute contribution from blocks below the diagonal
do iblock = 1, num_block_full
  call update_tri_block_boundaries(iblock, istart, iend, jstart, jend)
  do i = istart, iend
    do j = jstart, jend
      zij = z(j) - z(i)
      zijsq = zij * zij
      pot_ij = volfactor * (sqrpialpha * exp(-zijsq*alphasq) &
                            + pi * zij * erf(zij*alpha))
      V(j) = V(j) - q_elec(i) * pot_ij
      V(i) = V(i) - q_elec(j) * pot_ij
    end do
  end do
end do
end do

```