

```

! Compute contribution from blocks on the diagonal
do iblock = istart_block_diag, iend_block_diag
  call compute_diag_block_boundaries(iblock, istart, iend)
  do i = istart, iend
    do j = istart, iend
      (...)
      V_local(i) = V_local(i) - q_elec(j) * pot_ij
    end do
  end do
end do

! Compute contribution from blocks below the diagonal
do iblock = istart_block_full, iend_block_full
  call update_tri_block_boundaries(iblock, istart, iend, jstart, jend)
  do i = istart, iend
    do j = jstart, jend
      (...)
      V_local(j) = V_local(j) - q_elec(i) * pot_ij
      V_local(i) = V_local(i) - q_elec(j) * pot_ij
    end do
  end do
end do

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

```