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! 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
      call minimum_image_distance(x(i), y(i), z(i), x(j), y(j), z(j), drnorm2)
      if (drnorm2 < rcut_sq) then
        drnorm = sqrt(drnorm2)
        pot_ij = (erfc(alpha*drnorm) - erfc(eta*drnorm)) / drnorm
        V_local(i) = V_local(i) + q_elec(j) * pot_ij
      end if
    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
      call minimum_image_distance(x(i), y(i), z(i), x(j), y(j), z(j), drnorm2)
      if (drnorm2 < rcut_sq) then
        drnorm = sqrt(drnorm2)
        pot_ij = (erfc(alpha*drnorm) - erfc(eta*drnorm)) / drnorm
        V_local(j) = V_local(j) + q_elec(i) * pot_ij
        V_local(i) = V_local(i) + q_elec(j) * pot_ij
      end if
    end do
  end do
end do

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

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