Data structures of the wavelet program

Stefan Goedecker

Institut für Physik
Universität Basel, Switzerland

The molecule is covered by a global grid of dimensions 0:n1, 0:n2, 0:n3. The values n_1, n_2, n_3 are not input values but are calculated by the program as described below. The input parameter is the grid spacing hgrid. The real space location of a grid point (i1,i2,i3) is (i1*hgrid, i2*hgrid, i3*hgrid). The molecule is shifted by the program such that it is covered by this grid. There are three types of grid points. In addition there are local grids for the individual orbitals whose dimension is denoted in the program by the variables nl1:nu1, nl2:nu2, nl3:nu3. The local grids are always inside the global grid. Both the single global grid as well as the various local grids consist of

- grid points far from any atom that do not carry any basis function
- grid points in the coarse region carry a scaling function
- grid points in the fine resolution that carry in addition 7 wavelets.

The global grid points in the coarse region are all the grid points that satisfy the property that they are closer to some atom of type *ityp* than rcmult*radii_cf(ityp,1). The values of the array radii_cf are read from the second line of the pseudopotential files. The values radii_cf(*,1) give the assymptotic decay length of the wavefunction, $1/\sqrt{2\varepsilon_{HOMO}}$. The global grid points in the fine region are determined in the same way except that the distance criterion is rfmult*radii_cf(ityp,2). radii_cf(ityp,2) gives the radius where the pseudopotential of an atom of type ityp varies strongly. The factors rcmult and rfmult are read from the input file

The coarse and fine regions of the local grids are determined in the same way, except that in the above definitions not all the atoms are used but only the atoms belonging to the localization region of an orbital. So typically a localization region consists of a fine resolution region containing the few atoms forming the localization region and a much larger coarse resolution region. The determination of the localization region is at present based on the covalent radii of the atoms that are read from the second line of the pseudopotential files (third entry) and the parameter radlocmult that is read from the input file. Putting radlocmult to a very large value will results in completely delocalized orbitals. The array loregion specifies which atom centered spheres contribute to the localization region of a certain orbital. The various local grids are written into the files grid*.ascii that can be visualized with V_SIM.

The picture below shows a global grid for a silicon cluster

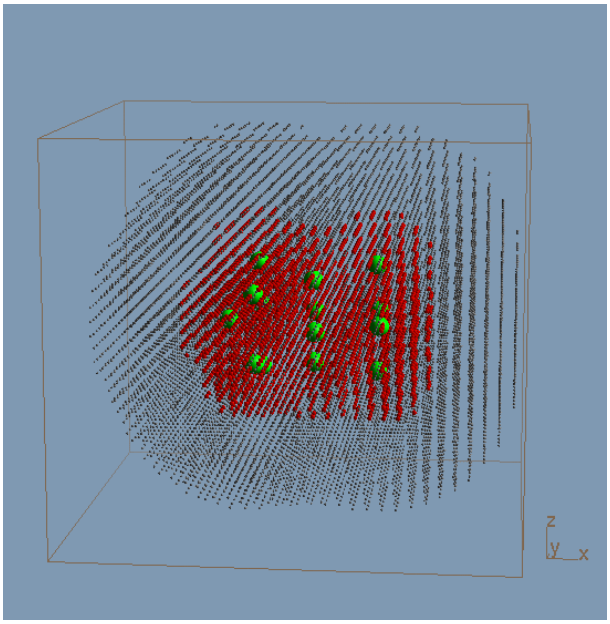

Figure 1: Grid around a silicon cluster. Atoms are big green spheres, grid points in the fine resolution region are shown in red, coarse resolution grid points in black.

Since not all grid points carry scaling functions and wavelets and since the coarse and fine resolution domains are irregular, the expansion coefficients of the wavefunctions are stored in compressed form. First the 3-dim grid is mapped onto an 1-dim array of length (n1+1) * (n2+1) * (n3+1). Then grid points carrying no basis functions are eliminated by compressing the data as shown below.

1 data structures in routines acting on a single orbital

Since there are typically lines along the x-axis whose grid points all carry basis functions, the compression is based on segments. In the present implementation, a segment can not contain the grid point of more than onle line. mseg_c and mseg_f give the number of segments for the scaling functions and wavelets. The compression of the wavelets is similar except that each box holds 7 data items. A compressed wavefunction consists of two vectors psi_c(mvctr_c) and psi_f(7,mvctr_f). keyg_c(1,*) and keyg_f(1,*) give the starting points of the segments and keyg_c(2,*) and keyg_f(2,*) give the end points of the segments in the vector of length (n1+1)*(n2+1)*(n3+1). keyv_c(*) gives the starting points in the compressed vector. A separate array for the end points is not necessary since there are no holes in the compressed data structure.

A single projector has exacly the same data structure. The coarse and fine regions for one projectors are given by the condition that the distance of the grid point to the atom to which the projector belongs is less than cpmult*radii_cf(*,2) and less than fpmult*radii_cf(*,2), where cpmult, fpmult are read from the input file.

2 data structures in routines acting on all orbitals

The scaling function and wavelet expansion coefficients of all the orbitals are contained in the array psi. The number of segments and the number of vector elements of all the orbitals is contained in the arrays nseg and nvctr. norb is the number of real space orbitals which is equal

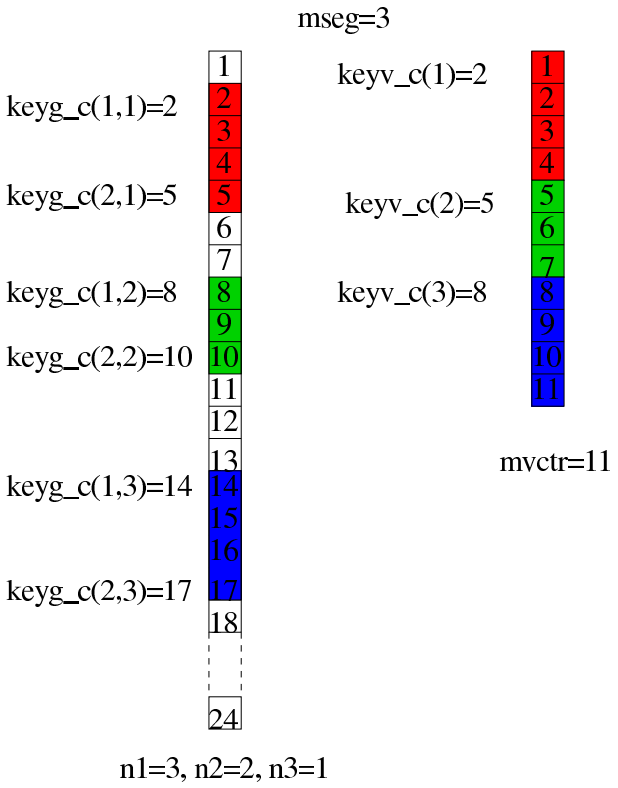

Figure 2: The data compression scheme. The subscripts _c has to be replaced by _f for the fine part.

to (half) of the number of electrons for a (non)-spinpolarized calculation.

```
do iorb=1,norb
   mseg_c=nseg(2*iorb-1)-nseg(2*iorb-2)   !number of coarse segments
   mseg_f=nseg(2*iorb  )-nseg(2*iorb-1)   !number of fine segments
   iseg_c=nseg(2*iorb-2)+1                !starting adress for coarse seg.
   iseg_f=nseg(2*iorb-1)+1                !starting adress for fine seg.
   mvctr_c= nvctr(2*iorb-1)-nvctr(2*iorb-2)    !# of coarse vector elem.
   mvctr_f=(nvctr(2*iorb  )-nvctr(2*iorb-1))/7 !# of fine vector elem./7
   ipsi_c=nvctr(2*iorb-2)+1            !starting address for coarse coef.
   ipsi_f=nvctr(2*iorb-1)+1            !starting address for fine coef.
   nl1=nbox_c(1,1,iorb) ; nu1=nbox_c(2,1,iorb)   ! local gridsize
   nl2=nbox_c(1,2,iorb) ; nu2=nbox_c(2,2,iorb)
   nl3=nbox_c(1,3,iorb) ; nu3=nbox_c(2,3,iorb)

!   call a routine that acts on a single orbital
   call singleorbital(n1,n2,n3,nl1,nu1,nl2,nu2,nl3,nu3,  &
              mseg_c,mvctr_c,keyg(1,iseg_c),keyv(iseg_c),   &
              mseg_f,mvctr_f,keyg(1,iseg_f),keyv(iseg_f),   &
              psi(ipsi_c),psi(ipsi_f),.............)
end do
```

For the projectors there is not one individual decriptor array (keyg, keyv) for each projector, but only one descriptor array per atom (with a separable part)

3 Miscalleneous

The atom types are specified by their pseudopotential. The parameters for the different pseudopotentials are contained in the the psppar.* files. The pseudopotential type follows in the input file after the 3 cartesian coordinates. For instance
0. 0. 0. Si_lda
means that the atom at the origin is described by the pseudopotential file psppar.Si_lda.

If the parameter calc_inp_wf in the input file is set to true an input guess for the wavefunctions is calculated. If calc_inp_wf is false initial wavefunctions are assumed to be in the wavefunction files and they are only read in from these files. If the wavefunctions in the wavefunction files were calculated with a different set of parameters (eg. different hgrid or rcmult) the readwave subroutine can do the necessary transformations.