Contents

A detailled description of the application of the finite difference method to the electronic structure has been given by Laaksonen et al in the case of an Hartree-Fock approcach[1].

1 Method

1.1 Conjugate gradient method

The solution of a linear systems of equation $\boldsymbol{A}|x>=-|b>$, where $\boldsymbol{A}$ is symmetric and positive definite, is equivalent to minimizing the quadratic function

$$f(|x>)=\frac{1}{2}<x|\boldsymbol{A}|x>+<b|x>+c, \tag{1}$$

with respect to the vector $|x>$.

2 The mesh

We deal with the problem by using finite differences on a cubic uniform grid, $\boldsymbol{r}_i$. In such ar representation, the Hamiltonian is sparse. We used second-order discretization for the Laplacian. In the framework of a finite differenc approach, the only nonvanishing matrix elements, $H_{ij}=<\boldsymbol{r}_i|\hat{H}|\boldsymbol{r}_j>$, are on the diagonal and between neighbouring points (2 in 1D, 4 in 2D and 6 in 3D):

$$H_{ij}=\begin{cases}\frac{1}{(\Delta\, x)^2+\Delta\, y)^2+\Delta\, z)^2}, & \text{if } i=j,\\ -\frac{1}{2(\Delta)^2}, & \text{if}|\boldsymbol{r}_i-\boldsymbol{r}_j|=\Delta,\\ 0, & \text{otherwise,}\end{cases} \tag{2}$$

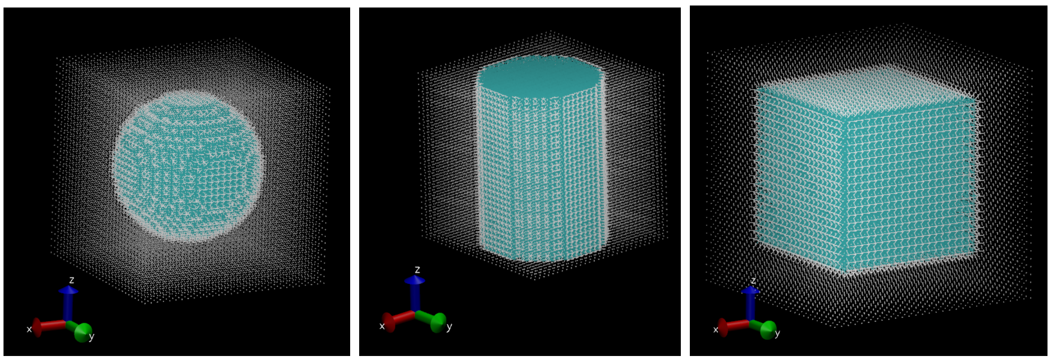
where $\Delta\, x$, $\Delta\, y$, et $\Delta\, z$ are the spacing between grid points.

Using Hartree atomic units, the Schrödinger we want to solve is

$$-\frac{1}{2}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{\mathrm{d}^2}{\mathrm{d}z^2}\right)\phi(x,y,z)+V(x,y,z)\phi(x,y,z)=\epsilon\phi(x,y,z) \tag{3}$$

For solving this equation, we resort to the finite difference method, a mesh-type approach[2, 3]. It consists to discretize the space in a finite set of locations in space so that to form a mesh:

$$\begin{aligned}(x,y,z) &\rightarrow (i,j,k), & (4)\\ \phi(x,y,z) &\rightarrow \phi_{i,j,k}, & (5)\\ & & (6)\end{aligned}$$



(a) Sphere (b) Cylinder (c) Cube

Figure 1: Definition of the "active" (blue) and "unactive" (white) domains. 3D Box 30 × 30 × 30 bohr radius; 30 × 30 × 30 nodes; radius of the computational domaine: 15 bohr radius.

with $x = i\Delta x$, $y = j\Delta y$, and $z = k\Delta z$.

Then, each node of the space obeys the equation

$$-\frac{1}{2}\phi''_{i,j,k} + V_{i,j,k}\phi_{i,j,k} = \epsilon\phi_{i,j,k}. \tag{7}$$

The principle of the finite difference method is to replace the derivatives in differential equations by approximations made up of a weighted sums of function values, derived using Taylor series expansions. The number of function values necessary to approximate a derivative at any node of the space depends on both the desired accuracy and the dimension. For example, at the lowest accurate approximation (three-point finite difference), in 3D, the second derivative of $\phi_{i,j,k}$ can be written as

$$\phi''_{i,j,k} = \frac{\phi_{i-1,j,k} - 2\phi_{i,j,k} + \phi_{i+1,j,k}}{(\Delta x)^2} + \frac{\phi_{i,j-1,k} - 2\phi_{i,j,k} + \phi_{i,j+1,k}}{(\Delta y)^2} + \frac{\phi_{i,j,k-1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}}{(\Delta z)^2} \tag{8}$$

For each node, the replacement of the derivatives by a sum of function value leads to a linear system of algebraic equations coupling the different values $\phi_{i,j,k}$:

$$-\frac{1}{2}\left(\frac{\phi_{i-1,j,k} - 2\phi_{i,j,k} + \phi_{i+1,j,k}}{(\Delta x)^2} + \frac{\phi_{i,j-1,k} - 2\phi_{i,j,k} + \phi_{i,j+1,k}}{(\Delta y)^2} + \frac{\phi_{i,j,k-1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}}{(\Delta z)^2}\right) + V_{i,j,k}\phi_{i,j,k} = \epsilon\phi_{i,j,k} \tag{9}$$

In the code, all informations about the mesh are stocked the data type `t_mesh` (defined in `global.f90`):

```
type t_mesh
   integer :: Nx,Ny,Nz,N,nactive,nunactive
   integer,allocatable :: list_bound(:,:),n_bound(:)  ! list_bound is linked with bound(:)
   double precision :: dx,dy,dz,dv
   type(t_box)::box
   integer :: dim
   integer::nbound
   type(t_point),allocatable::bound(:)
   type(t_ijk_to_idx),allocatable::ijk_to_idx(:,:,:)  ! from (i,j,k) -> n
   type(t_node),allocatable::node(:)
end type t_mesh
```

Different kinds of parameters are necessary to define the mesh: the dimension (1D, 2D or 3D), shape of the box(sphere, cube, ...), size of the box(L_x, L_y, L_z), number of nodes (N_x, N_y, N_z), ...

The mesh spacings, Δx, Δy and Δz, are then given by $\Delta\alpha = L_\alpha/(N_\alpha + 1)$.

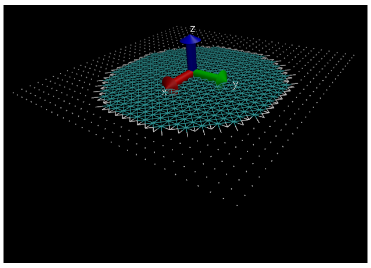


Figure 2: Definition of the "active" (blue) and "unactive" (white) domains. 2D Box 30×30 bohr radius; 30×30 nodes; radius of the computational domaine: 15 bohr radius.

The mesh is defined by calling the subroutine `new_mesh(mesh,param)` (in `mesh.f90`). The mesh, containing $N = N_x \times N_y \times N_z$ nodes, consists in two kind of nodes: the "active" nodes, belonging to the computational domain, and the "unactive" ones, belonging to the boundaries domain (figs. 1 and 2). The "active" nodes are the nodes where we will compute quantities such as wavefunctions, potentials, ... while the "unactive" nodes are the nodes where all these quantities are constant. Example of "unactive" nodes is the nodes located in the outer edge of the box defining the shape of the space we consider. At these locations, the value of the wavefunction is zero in the case of isolated systems. The type of any node of the space is determined by the subroutine `set_nodes(mesh)`:

- if the node (i,j,k) belongs to the computational domain, an single positive index n is assigned to the node; each index n corresponds to an single set (i,j,k) of the space.

$$(x,y,z) \quad \rightarrow (i,j,k) \rightarrow \quad n, \tag{10}$$
$$\phi(x,y,z) \quad \rightarrow \phi_{i,j,k} \rightarrow \quad \phi_n, \tag{11}$$

  The total number of nodes inside the computational domain is n_{active}.

- if the node (i,j,k) belongs to the boundaries domain, its index n is set to -1.

The computational and boundaries domains are defined thanks to parameters decribing the shape and the size of the computational box (`mesh%box%shape`, `mesh%box%center`, `mesh%box%radius`)

From equations (9) and by using the application $(x,y,z) \rightarrow (i,j,k) \rightarrow n$, solving the Schrödinger equation (3) is equivalent to solve an eigenvalues problem $H|\phi>=\epsilon|\phi>$; the vector $|\phi>$ is an eigenvector to be determined, corresponding to the eigenvalue ϵ.

For each node (i,j,k), the list of neighbors ($(i\pm1,j,k)$, $(i,j\pm1,k)$, $(i,j,k\pm1)$ in the case given here) involved in equations (9) is given by the matrix `mesh%node(nactive)%list_neighbors(:)` (`mesh%node(nactive)%n_neighbors` contains the number of neighbors for each node (i,j,k)). These lists are set in the subroutine `compute_list_neighbors(mesh)`.

3 Electrostatic potential

There two ways to compute the electrostatic potential of the charge distribution, $\rho(\boldsymbol{r})$, of the electron in the system:

- by solving the Poisson equation, $\nabla U(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r})$ (Hartree a. u.),
- by solving the integral equation, $U(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}'\rho(\boldsymbol{r}')\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}$.

Solving the integral equation is the simplest way to proceed but it is also the most inefficient because it needs to integrate the equation for each point belonging to the grid.

Using the Poisson equation is a more efficient way to proceed. In the framework of the finite difference method, in three dimensions (3D), the Poisson equation has the form

$$\frac{U_{i-1,j,k} - 2U_{i,j,k} + U_{i+1,j,k}}{(\Delta x)^2} + \frac{U_{i,j-1,k} - 2U_{i,j,k} + U_{i,j+1,k}}{(\Delta y)^2} + \frac{U_{i,j,k-1} - 2U_{i,j,k} + U_{i,j,k+1}}{(\Delta z)^2} = -4\pi\rho_{i,j,k}. \tag{12}$$

For each active node, the replacement of the second derivative of the electrostatic potential by a sum of functions leads to a linear systems of algebrais equations coupling the different value $U_{i,j,k}$,

$$L|U >= -4\pi|\rho > . \tag{13}$$

L is the Laplace matrix.

Note that for the active nodes located at the edge of the active domain, the replacement of the second derivative by a sum of function needs to take into account the unactive nodes located at the edge of the unactive. For example, for the node (i, j, k),

$$\frac{U^*_{i-1,j,k} - 2U_{i,j,k} + U_{i+2,j,k}}{(\Delta\, x)^2} + \frac{U_{i,j-1,k} - 2U_{i,j,k} + U_{i,j+1,k}}{(\Delta\, y)^2} + \frac{U_{i,j,k-1} - 2U_{i,j,k} + U_{i,j,k+1}}{(\Delta\, z)^2} = -4\pi\rho_{i,j,k} \tag{14}$$

the node $U^*_{i-1,j,k}$ belongs to the unactive domain and imposes a boundary condition. Note that only a part of the unactive domain is involved in the boundary conditions. This part of the unactive domain is noted Ω in the following. The unactive nodes involved in the boundary conditions are listed in the data type `t_node`: for each active node, the integer `mesh%node(:)%n_bound` gives the number of neigbors unactive nodes contributing to the boundary conditions (their index is given in `mesh%node(:)%list_bound(:)`).

Then

$$\frac{-2U_{i,j,k} + U_{i+2,j,k}}{(\Delta\, x)^2} + \frac{U_{i,j-1,k} - 2U_{i,j,k} + U_{i,j+1,k}}{(\Delta\, y)^2} + \frac{U_{i,j,k-1} - 2U_{i,j,k} + U_{i,j,k+1}}{(\Delta\, z)^2} = -4\pi\rho_{i,j,k} - \frac{U^*_{i-1,j,k}}{(\Delta\, x)^2} \tag{15}$$

$$-2\left(\frac{1}{(\Delta\, x)^2} + \frac{1}{(\Delta\, y)^2} + \frac{1}{(\Delta\, z)^2}\right) U_{i,j,k} + \frac{U_{i+2,j,k}}{(\Delta\, x)^2} + \frac{U_{i,j-1,k}}{(\Delta\, y)^2} + \frac{U_{i,j+1,k}}{(\Delta\, y)^2} + \frac{U_{i,j,k-1}}{(\Delta\, z)^2} + \frac{U_{i,j,k+1}}{(\Delta\, z)^2} = -4\pi\rho_{i,j,k} - \frac{U^*_{i-1,j,k}}{(\Delta\, x)^2} \tag{16}$$

$$L|U >= -4\pi|\rho > -|b > . \tag{17}$$

$|b >$ is the vector containing the boundary conditions, $i..e$, the values of the electrostatic potential at the edge of th e active domain.

Now the question is: how to get the values of the electrostatic potential at the unactive point edge of the unactive domain in

4 Structure of the input file

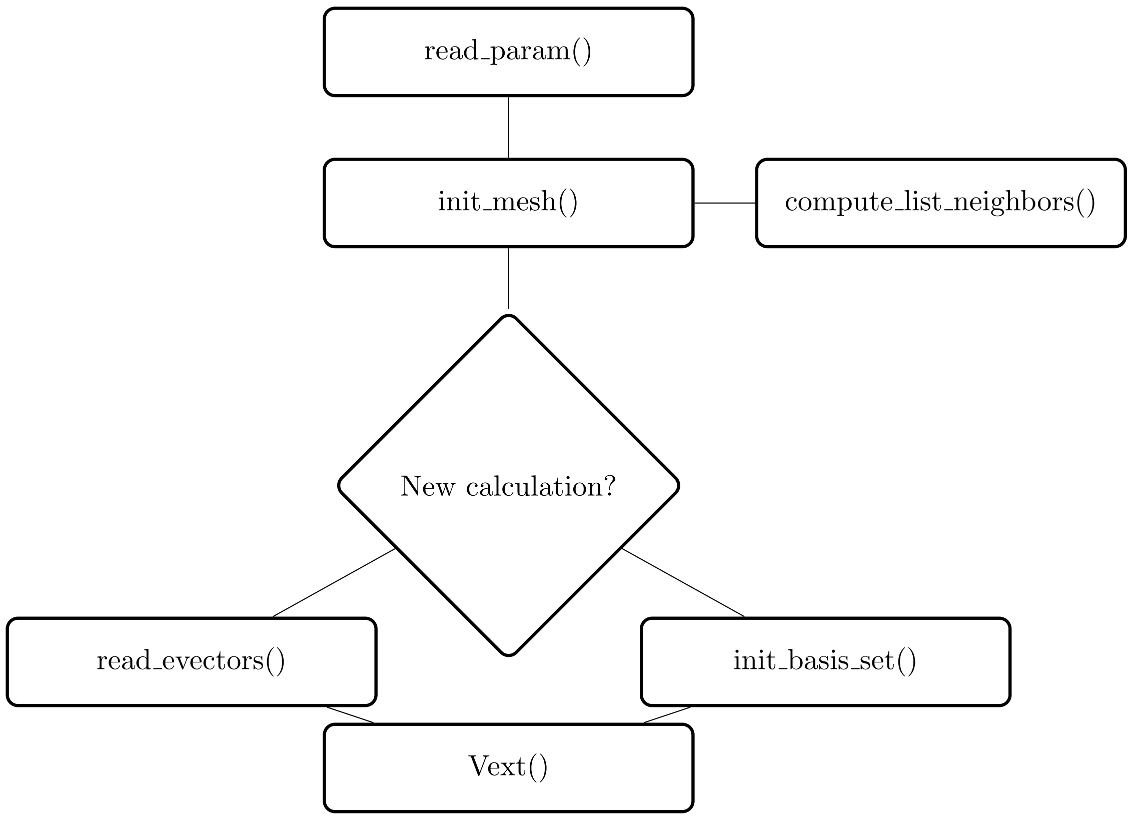
The input file is provided directly from the command line: `./Hbinitio.x inp_davidson` for example.
It must be ended by the line `cmd=end` to indicate the end of the file.

5 Structure of the code

Algorithm 1: read_param(syst)

```
Data: this text
Result: how to write algorithm with LaTeX2e
initialization;
while not at end of this document do
    while .not.(is_iostat_end(param%ieof))).and.(.not.(end_loop) do
        read(2,'(A)') line call line$_parser(line, nfield, field)print*, nfield,' -- >', (trim(field(i)), i = 1, nfield)callparse_line(param, field, nfield, end_loop, systprint*, "end_loop = ", end_loopenddo$ end
        read current;
        if understand then
            go to next section;
            current section becomes this one;
        else
            go back to the beginning of current section;
        end
    end

```



6 Dealing with the perturbation

6.1 Real-space representation of the resolvent of the Hamiltonian, $\hat{H}$

A way to compute the electron density, $n(\boldsymbol{r})$, is to resort to the identity relating the density matrix of a system, $\rho(\boldsymbol{r}, \boldsymbol{r}')$, with its one-electron Green's function:

$$G(\boldsymbol{r}, \boldsymbol{r}'; \epsilon) =< \boldsymbol{r}|\hat{G}(\epsilon)|\boldsymbol{r}' >=< \boldsymbol{r}|\frac{1}{\epsilon - \hat{H}}|\boldsymbol{r}' > \tag{18}$$

$n(\boldsymbol{r}) = \rho(\boldsymbol{r}, \boldsymbol{r})$

Baroni and Giannozzi[4] introduced a Green's function method which employs the finite difference and a real-space grid.

Using the Green's method needs to calculate the inverse of $(\epsilon - \hat{H})$ which may be an huge task. Iterative algorithms, such as the Davidson's one, used to solve elliptic partial differential equations could in principle be used to calculate the inverse of $(\epsilon - \hat{H})$ (in the Davidson's method they are used to compyte de $|delta>$ vector from the residual). However, for the Green's method, we don't need to get the *full* inverse matrix but only the diagonal element of the inverse.

Haydock, Heine and Kelly[5, 6] developped a convenient way to compute a *single* diagonal element of the Green's function: the recursion method. In the recursion method, diagonal elements of the Green's function, $<\phi_0|\hat{G}|\phi_0>$, are expressed in terms of a continuous fraction whose coefficients are calculated from a chain of orthogonal states recursively generated from $|\phi_0>$:

7 Sources

```
#! /bin/bash
####SBATCH -p public
#SBATCH -p grant -A g2018a7
###SBATCH -p grantgpu -Ag1018a7
#SBATCH -n 64 -tasks-per-node=64
#SBATCH -t 2:00:00              # Le job sera tue au bout de 1h
####SBATCH --mail-user=herve.bulou@ipcms.unistra.fr
#####SBATCH --mem=4096               # Quantite memoire demandee par noeud en Mo (unite obligat


export OMP_NUM_THREADS=64
time ./Hbinitio.x


module time_tracking
  implicit none
  type t_time
     real :: start,end,start_loc,end_loc
  end type t_time
contains
  ! ----------------------------------------------
  subroutine time_tracking_init(time_spent)
    implicit none
    type(t_time)::time_spent
    call cpu_time(time_spent%start)
    open(unit=1,file="dbg.dat",form='formatted',status='unknown')
    write(1,*)
    close(1)
  end subroutine time_tracking_init
  subroutine time_tracking_write(iloop,time_spent,text)
    integer :: iloop
    type(t_time)::time_spent
    character (len=*) :: text
    open(unit=1,file="dbg.dat",form='formatted',status='unknown',access='append')
    write(1,'(A50,I4,F12.6,F12.6,F12.6)') text,iloop,time_spent%end_loc,&
         time_spent%start_loc,time_spent%end_loc-time_spent%start_loc
    close(1)
  end subroutine time_tracking_write
end module time_tracking

  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
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  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
program Hbinitio
  !$ use OMP_LIB
  use time_tracking
  implicit none
!  include 'mpif.h'
  type t_GramSchmidt
     integer :: nindep
     integer :: ndep ! number of linear dependencies discovered
  end type t_GramSchmidt
  type t_mesh
     integer :: Nx,Ny,Nz,N
     integer,allocatable :: list_neighbors(:,:),n_neighbors(:)
     double precision :: dx,dy,dz,dv
     double precision :: center(3)
  end type t_mesh
  type(t_mesh) :: mesh
  type t_cvg
     integer,allocatable:: list_cvg(:)
     integer :: ncvg
     double precision :: ETA
     integer :: nvec_to_cvg
  end type t_cvg
  type(t_cvg) :: cvg
  type(t_time) :: time_spent
  type t_param
     logical::restart
     integer::ieof
     integer::loopmax
     integer::nvecini
     integer::nvecmax
     integer::Nx
     integer::nvec_to_cvg
     double precision :: ETA
     double precision::box_width
  end type t_param
  type(t_param)::param
  integer :: nvec
  integer,parameter :: seed = 86456
  double precision,allocatable :: V(:,:) ! wavefunctions
  double precision,allocatable :: Sprev(:),dS(:) ! eigenvalues
  double precision,allocatable :: pot_ext(:) ! external potential
  integer :: iloop
  character (len=1024) :: filecube
  character (len=1024)::line
  integer :: i
```

```
!  integer::ierr,my_id,num_procs
  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

  call time_tracking_init(time_spent)

!  call mpi_init(ierr )
!  call MPI_COMM_RANK (MPI_COMM_WORLD, my_id, ierr)
!  call MPI_COMM_SIZE (MPI_COMM_WORLD, num_procs, ierr)

  call read_param(param)
  call init_mesh(mesh,param)

!  nvecini=2
  nvec=param%nvecini
  allocate(V(mesh%N,nvec))
!  param%restart=.TRUE.
!  param%restart=.FALSE.
  if (.not.(param%restart))   then
     print *,"new calculation"
     call init_basis_set(V,nvec,seed,mesh)
  else
     print *,'restart an old calculation'
     call read_evectors(V,mesh,nvec)
  end if
  allocate(pot_ext(mesh%N))
  call Vext(mesh,pot_ext)

  open(unit=1,file="eigenvalues.dat",form='formatted',status='unknown'); write(1,*);  close(1)

  iloop=1
  cvg%ncvg=0
  cvg%nvec_to_cvg=param%nvec_to_cvg
  cvg%ETA=param%ETA
  allocate(Sprev(param%nvecini))
  allocate(dS(param%nvecini))
  Sprev(:)=0.0
  dS(:)=0.0
  do while((iloop.le.param%loopmax).and.(cvg%ncvg.lt.cvg%nvec_to_cvg))
     write(*,'(A)') 'Main > ########################################'
     write(*,'(A,I4,A)') 'Main > ############ scf loop=',iloop,' ############'
     write(*,'(A)') 'Main > ########################################'
     call davidson(nvec,V,mesh,param%nvecini,iloop,cvg,pot_ext,time_spent)
  end do
  call save_evectors(V,mesh,param%nvecini)
  do i=1,param%nvecini
     write(filecube,'(a,i0,a)') 'evec',i,'.cube'
     call norm(mesh,V(:,i))
     call save_cube(V(:,i),filecube,mesh)
  end do
  deallocate(V)
  deallocate(Sprev)
  deallocate(dS)
  deallocate(pot_ext)
  call free_mesh(mesh)
  call cpu_time(time_spent%end)
  if (cvg%ncvg.ge.cvg%nvec_to_cvg) print *,'Main > Job DONE !'
  print '("Main > Total Time = ",e16.6," seconds.")',time_spent%end-time_spent%start
!  call mpi_finalize(ierr)
  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
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  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
contains
  ! --------------------------------------------------------------------------------------
  !
  !              read_param()
  !
  ! --------------------------------------------------------------------------------------
  subroutine read_param(param)
    implicit none
    type(t_param)::param
    integer::lline,eqidx
    double precision, parameter :: pi=3.1415927

    param%ieof=0
    param%loopmax=1000
    param%restart=.FALSE.
    param%nvecini=20
    param%nvecmax=41
    param%Nx=30
    param%nvec_to_cvg=20
    param%ETA=1.0e-3
    param%box_width=pi/sqrt(2.0)
    open(unit=1,file='inp',form='formatted')
    do while(.not.(is_iostat_end(param%ieof)))
       read(1,*,iostat=param%ieof) line
       lline=len_trim(line)
       eqidx=index(line,"=")
       print *,'###',eqidx,lline
       if(line(1:eqidx-1).eq."restart") then
          if(line(eqidx+1:lline).eq.'.TRUE.') then
             param%restart=.TRUE.
          else
             param%restart=.FALSE.
          end if
       end if
       if(line(1:eqidx-1).eq."loopmax") then
          read(line(eqidx+1:lline),*) param%loopmax
       end if
       if(line(1:eqidx-1).eq."nvecini") then
          read(line(eqidx+1:lline),*) param%nvecini
       end if
       if(line(1:eqidx-1).eq."nvecmax") then
```

```
        read(line(eqidx+1:lline),*) param%nvecmax
     end if
     if(line(1:eqidx-1).eq."Nx") then
        read(line(eqidx+1:lline),*) param%nx
     end if
     if(line(1:eqidx-1).eq."ETA") then
        read(line(eqidx+1:lline),*) param%ETA
     end if
     if(line(1:eqidx-1).eq."nvec_to_cvg") then
        read(line(eqidx+1:lline),*) param%nvec_to_cvg
     end if
     if(line(1:eqidx-1).eq."box_width") then
        read(line(eqidx+1:lline),*) param%box_width
     end if
     line=''
  end do
  close(1)


  print *,'#restart=',param%restart
  print *,'#loopmax=',param%loopmax
  print *,'#nvecini=',param%nvecini
  print *,'#nvecmax=',param%nvecmax
  print *,'#ETA=',param%ETA
  print *,'#nvec_to_cvg=',param%nvec_to_cvg
  print *,'#box_width=',param%box_width
  print *,'#Nx=',param%nx
  print *,'#dh=',param%box_width/(param%Nx+1)

end subroutine read_param
! --------------------------------------------------------------------------------------
!
!               save_evectors()
!
! --------------------------------------------------------------------------------------
subroutine save_evectors(V,m,nvecini)
  implicit none
  type(t_mesh)::m
  double precision :: V(:,:)
  integer::nvecini,i,j
  open(unit=1,file="evectors.dat",form='formatted',status='unknown')
  do i=1,m%N
     write(1,*) (V(i,j),j=1,nvecini)
  end do
  close(1)
end subroutine save_evectors
! --------------------------------------------------------------------------------------
!
!               read_evectors()
!
! --------------------------------------------------------------------------------------
subroutine read_evectors(V,m,nvecini)
  implicit none
  type(t_mesh)::m
  double precision :: V(:,:)
  integer::nvecini,i,j
  open(unit=1,file="evectors.dat",form='formatted',status='unknown')
  do i=1,m%N
     read(1,*) (V(i,j),j=1,nvecini)
  end do
  close(1)
end subroutine read_evectors
! --------------------------------------------------------------------------------------
!
!              norm()
!
! --------------------------------------------------------------------------------------
subroutine  norm(m,evec)
  implicit none
  double precision :: evec(:),normloc
  double precision, external :: ddot
  type(t_mesh)::m
  normloc=sqrt(m%dv*ddot(m%N,evec(:),1,evec(:),1))
  call dscal(m%N,normloc,evec(:),1)
end subroutine norm
! --------------------------------------------------------------------------------------
!
!              Vext()
!
! --------------------------------------------------------------------------------------
subroutine Vext(m,pot_ext)
  implicit none
  type(t_mesh) :: m
  double precision :: pot_ext(:)
  double precision :: pts(3),rsqr

  character (len=1024) :: filename
  integer :: i,j,k,nn
  do k=1,m%Nz
     pts(3)=k*m%dz
     do i=1,m%Nx
        pts(1)=i*m%dx
        do j=1,m%Ny
           pts(2)=j*m%dy
           rsqr=(pts(1)-m%center(1))**2+(pts(2)-m%center(2))**2+(pts(3)-m%center(3))**2
           nn=j+(i-1)*m%Ny+(k-1)*m%Ny*m%Nx
           pot_ext(nn)=10*rsqr
        end do
     end do
  end do
  filename='pot_ext.cube'
  call save_cube(pot_ext,filename,m)
  !stop
end subroutine Vext
! --------------------------------------------------------------------------------------
!
```

```
!              DAVIDSON()
!
! -------------------------------------------------------------------------------------
subroutine davidson(nvec,V,m,nvecini,iloop,cvg,pot_ext,time_spent)
  implicit none
  integer :: nvec,nvecini,iloop
  double precision,allocatable :: V(:,:),pot_ext(:)
  type(t_mesh) :: m
  type(t_cvg)::cvg
  type(t_time)::time_spent

  double precision,allocatable :: S(:) ! eigenvalues
  double precision,allocatable :: T(:,:) ! reduced matrix T
  double precision,allocatable :: VRitz(:,:) ! Ritz's vectors
  double precision,allocatable :: residual(:,:) ! residual
  double precision,allocatable :: delta(:,:) ! delta vectors
  double precision,allocatable :: Vnew(:,:) ! Vnew
  integer :: i
  integer :: ndelta
  integer :: newnvec
  type(t_GramSchmidt)::GS
  ! T (reduced matrix) computing
  allocate(T(nvec,nvec))
  call cpu_time(time_spent%start_loc)
  call compute_T(T,V,nvec,m,pot_ext)
  call cpu_time(time_spent%end_loc)
  call time_tracking_write(iloop,time_spent,'Davidson -> compute_T')

  ! Diagonatilzation of T
  allocate(S(nvec))

  call cpu_time(time_spent%start_loc)
  call diagonalization(S,T,nvec)
  call cpu_time(time_spent%end_loc)
  call time_tracking_write(iloop,time_spent,'Davidson -> Diagonalization')


  dS(:)=S(1:nvecini)-Sprev(:)
  Sprev(:)=S(1:nvecini)
  do i=1,nvecini
     write(*,'(A,I6,A,F12.6,A,E12.2,A)') 'Main > Eigenvalue(',i,'): ',S(i),'(',dS(i),')'
  end do
  !call cpu_time(inter)
  open(unit=1,file="eigenvalues.dat",form='formatted',status='unknown',access='append')
  write(1,*) iloop,S(1:nvecini)
  close(1)
  ! computation of the Ritz's vectors
  allocate(VRitz(m%N,nvec))

  call cpu_time(time_spent%start_loc)
  call Ritz(VRitz,V,T,nvec)
  call cpu_time(time_spent%end_loc)
  call time_tracking_write(iloop,time_spent,'Davidson -> Diagonalization')
```

```
! computation of residual
allocate(residual(m%N,nvec))
allocate(cvg%list_cvg(nvec))
cvg%list_cvg(:)=0
cvg%ncvg=0


call cpu_time(time_spent%start_loc)
call compute_residual(residual,VRitz,S,nvec,cvg,m,pot_ext)
call cpu_time(time_spent%end_loc)
call time_tracking_write(iloop,time_spent,'Davidson -> Residual')

! computation of delta
allocate(delta(m%N,nvec))
delta(:,:)=0.0
!call cpu_time(inter)

call cpu_time(time_spent%start_loc)
call compute_delta(delta,residual,S,nvec,cvg,m,ndelta,pot_ext)
call cpu_time(time_spent%end_loc)
call time_tracking_write(iloop,time_spent,'Davidson -> Delta')


deallocate(V)
allocate(V(m%N,nvec+ndelta))
V(:,1:nvec)=VRitz(:,:)
print *,'ndelta=',ndelta
print *,'nvec=',nvec
V(:,nvec+1:nvec+ndelta)=delta(:,:ndelta)
allocate(Vnew(m%N,nvec+ndelta))
newnvec=nvec+ndelta
GS%nindep=nvec
!call cpu_time(inter)
call GramSchmidt(Vnew,V,newnvec,m,GS)
! call cpu_time(inter2);     call dbg(iloop,inter,inter2,'GS')

print *,'Main > ',GS%ndep,newnvec

deallocate(V)
if(newnvec.le.param%nvecmax) then
   nvec=newnvec
else
   print *,'Main > restart from nvecini'
   nvec=nvecini
end if
allocate(V(m%N,nvec))
V(:,:)=Vnew(:,1:nvec)

!call check_ortho(V,nvec,m)
print *,'Main > New size of the basis ',nvec
iloop=iloop+1
```

```
    deallocate(S)
    deallocate(T)
    deallocate(VRitz)
    deallocate(residual)
    deallocate(delta)
    deallocate(Vnew)
    deallocate(cvg%list_cvg)
  end subroutine davidson
  ! ---------------------------------------------------------------------------------------
  !
  !              SAVE_CUBE()
  !
  ! ---------------------------------------------------------------------------------------
  subroutine save_cube(data,filename,m)
    implicit none
    double precision :: data(:)
!    integer :: idxmin,idxmax
    type(t_mesh) :: m
    character (len=1024) :: filename

    character(len=*),parameter :: FMT1='(I5,3F12.6)'
    integer :: i,j,k,nn,ifield

    open(unit=1,file=filename,form='formatted',status='unknown')
    write(1,*) ' Cubefile created from Hbinitio.f90 calculation'
    write(1,*) ' H. Bulou, November 2018'
    write(1,FMT1) 1,0.0,0.0,0.0
    write(1,FMT1) m%Nx,m%dx,0.0,0.0
    write(1,FMT1) m%Ny,0.0,m%dy,0.0
    write(1,FMT1) m%Nz,0.0,0.0,m%dz
    write(1,'(I5,4F12.6)') 1,1.0,0.0,0.0,0.0
    do k=1,m%Nz
       ifield=0
       do i=1,m%Nx
          do j=1,m%Ny
             nn=j+(i-1)*m%Ny+(k-1)*m%Ny*m%Nx
             write(1,'(E13.5)',advance='no') data(nn)
             ifield=ifield+1
             if (mod(ifield,6).eq.0) then
                ifield=0
                write(1,*)
             end if
          end do
       end do
       write(1,*)
    end do
    close(1)
  end subroutine save_cube

  ! ---------------------------------------------------------------------------------------
  !
  !              COMPUTE_DELTA()
  !
  ! -----------------------------------------------------------------------------------------
  subroutine compute_delta(delta,r,lambda,nvec,cvg,m,ndelta,pot_ext)
    ! INPUT: the residual |r>, the Ritz's vectors |VRitz>, the eigenvalues lambda
    ! OUTPUT : the correction |delta> to improve the  Ritz's vectors so that to
    !          minimize the residual
    implicit none
    type(t_mesh)::m
    double precision :: lambda(:),r(:,:),delta(:,:),pot_ext(:)
    integer :: nvec,ndelta
    type(t_cvg)::cvg

    double precision, external :: ddot
    double precision, parameter::alpha=1.0,beta=0.0
    double precision, allocatable :: normloc
!    double precision, allocatable :: Dinv(:,:)
    integer :: i,j
    double precision :: deltasqr

    deltasqr=m%dx**2
    print *,'Delta > ---------------------'
    print *,'Delta > --- compute_delta ---'
    print *,'Delta > ---------------------'
    !delta(:,:)=0.0
   ! allocate(Dinv(m%N,m%N))
  !  Dinv(:,:)=0.0
    ndelta=0
    do i=1,nvec
       if(cvg%list_cvg(i).eq.0) then
          ndelta=ndelta+1
          do j=1,m%N
             delta(j,ndelta)=r(j,ndelta)/((3.0/deltasqr+pot_ext(j))-lambda(i))
!             Dinv(j,j)=1.0/((3.0/deltasqr+pot_ext(j))-lambda(i))
          end do
          ! see Victor Eijkhout in "Introduction to scientific and technical computing" edited b
          ! Chap 15 Libraries for Linear Algebra
          ! to get a comprehensive way to use dgemv
!          call dgemv('N',m%N,m%N,alpha,Dinv,m%N,r(:,ndelta),1,beta,delta(:,ndelta),1)
          !norm=sqrt(ddot(m%N,delta(:,i),1,delta(:,i),1))
          !write(*, '(A10,I4,A2,E12.6)',advance='no') ' Delta > delta(',i,')=',norm
          !delta(:,ndelta)=delta(:,ndelta)+VRitz(:,ndelta)
          normloc=1.0/sqrt(ddot(m%N,delta(:,ndelta),1,delta(:,ndelta),1))
          call dscal(m%N,normloc,delta(:,ndelta),1)
       end if
    end do
    !deallocate(Dinv)
    print *,'Delta > ',ndelta,' new vector(s)'
  end subroutine compute_delta


  ! -----------------------------------------------------------------------------------------
  !
  !               COMPUTE_RESIDUAL()
  !
```

```
! -----------------------------------------------------------------------------
subroutine compute_residual(r,VRitz,S,nvec,cvg,m,pot_ext)
  implicit none
  type(t_mesh)::m
  integer :: nvec
  double precision :: r(:,:),VRitz(:,:),S(:),pot_ext(:)
  type(t_cvg) :: cvg

  integer :: i,j,k
  double precision :: normloc
  double precision, external :: ddot
  double precision :: deltasqr

  print *,'Residual > -----------------------'
  print *,'Residual > --- compute residual ---'
  print *,'Residual > -----------------------'
  deltasqr=m%dx**2
  r(:,:)=0.0
  cvg%ncvg=0
  do j=1,nvec
     do i=1,m%N
        r(i,j)=(3.0/deltasqr+pot_ext(i))*VRitz(i,j)
        do k=1,m%n_neighbors(i)
           r(i,j)=r(i,j)-0.5*VRitz(m%list_neighbors(i,k),j)/deltasqr
        end do
        r(i,j)=r(i,j)-S(j)*VRitz(i,j)
     end do
     normloc=ddot(m%N,r(:,j),1,r(:,j),1)
     write(*,'(A,I4,A,E12.4,A,E12.4)',advance='no') 'Residual > r(',j,')= ',normloc,'/',cvg%ET
     if (normloc.lt.cvg%ETA) then
        cvg%ncvg=cvg%ncvg+1
        cvg%list_cvg(j)=1
        write(*,*) '--> converged'
     else
        write(*,*)
     end if

  end do
end subroutine compute_residual

! -----------------------------------------------------------------------------
!
!              RITZ()
!
! -----------------------------------------------------------------------------
subroutine Ritz(Vout,Vin,y,nvec)
  implicit none
  double precision :: Vin(:,:),Vout(:,:),y(:,:)
  integer :: nvec

  integer :: i,j
  print *,'Ritz > --------------'
  print *,'Ritz > --- Ritz() ---'
  print *,'Ritz > --------------'
  do i=1,nvec
     Vout(:,i)=y(1,i)*Vin(:,1)
     do j=2,nvec
        Vout(:,i)=Vout(:,i)+y(j,i)*Vin(:,j)
     end do
  end do
end subroutine Ritz


! ---------------------------------------------------------------------------------------
!
!             DIAGONALIZATION()
!
! ---------------------------------------------------------------------------------------
subroutine diagonalization(S,H,N)
  implicit none
  integer :: N
  double precision :: H(:,:),S(:)

  integer :: lwork,info
  integer :: lwmax
  double precision,allocatable::work(:)
  parameter(lwmax=100000)
  allocate(work(lwmax))
  lwork=-1
  call  dsyev('vectors','Upper',N,H,N,S,work,lwork,info)
  lwork=min(lwmax,int(work(1)))
  if (lwork.ge.lwmax) then
     write(*,*) 'Diagonalization > WARNING info = ',info
     write(*,*) 'Diagonalization > WARNING lwork=',lwork
     write(*,*) 'Diagonalization > WARNING size of work(1)',int(work(1))
     stop
  end if
  call  dsyev('vectors','Upper',N,H,N,S,work,lwork,info)
  if(info.gt.0) then
     write(*,*) "Diagonalization > WARNING The algorithm computing failed"
     stop
  end if
  deallocate(work)
end subroutine diagonalization


! ---------------------------------------------------------------------------------------
!
!             COMPUTE_T()
!
! ---------------------------------------------------------------------------------------
subroutine compute_T(T,V,nvec,m,pot_ext)
  implicit none
  double precision,allocatable :: V(:,:),T(:,:),pot_ext(:)
  integer :: nvec
  type(t_mesh)::m
```

```
    integer :: i,j,k,l
    double precision :: deltasqr,acc
    double precision, parameter::alpha=0.0
!    double precision::beta

    deltasqr=m%dx**2
    !$OMP PARALLEL private(acc)
    !$OMP DO
    do j=1,nvec
       do i=1,nvec ! Tij
          T(i,j)=0.0
          do k=1,m%N
             acc=(3.0/deltasqr+pot_ext(k))*V(k,j) ! the potential will be added here
             do l=1,m%n_neighbors(k)
                acc=acc-0.5*V(m%list_neighbors(k,l),j)/deltasqr
!                print *, omp_get_thread_num(),i,j,k,l
             end do
             T(i,j)=T(i,j)+V(k,i)*acc
!             print *,' -> ',omp_get_thread_num(),i,j,T(i,j)
          end do
!          print *,omp_get_thread_num(),i,j,T(i,j)
       end do
    end do
    !$OMP END DO
    !$OMP END PARALLEL
!    stop
  end subroutine compute_T


  ! ---------------------------------------------------------------------------------------
  !
  !               INIT_BASIS_SET()
  !
  ! ---------------------------------------------------------------------------------------
  subroutine init_basis_set(V,nvec,seed,m)
    implicit none
    integer :: nvec,seed
    double precision,allocatable :: V(:,:)
    type(t_mesh)::m

    double precision, external :: ddot
    double precision ::normloc
    integer :: i,j
    double precision,allocatable :: Vdump(:,:)
    type(t_GramSchmidt) :: GS

    allocate(Vdump(m%N,nvec))
    call srand(seed)
    do i=1,nvec
       do j=1,m%N
          Vdump(j,i)=rand()
       end do
    end do
    do i=1,nvec
       normloc=ddot(m%N,Vdump(:,i),1,Vdump(:,i),1)
       normloc=1.0/sqrt(normloc)
       call dscal(m%N,normloc,Vdump(:,i),1)
    end do
    GS%nindep=1
    call GramSchmidt(V,Vdump,nvec,m,GS)

    deallocate(Vdump)
  end subroutine init_basis_set
  ! ------------------------------------------------
  ! Ref.: D. G. Clayton "Gram-Schmidt Orthogonalization", J. Roy. Stat. Soc. C 20, 335 (1971)
  subroutine GramSchmidt(Vout,Vin,nvec,m,GS)
    implicit none
    integer ::  nvec
    double precision,allocatable :: Vin(:,:),Vout(:,:)
    type(t_mesh)::m
    type(t_GramSchmidt) :: GS

    integer :: i,k,i0
    double precision, parameter :: ETA=1.0e-6
    double precision,allocatable :: a(:)
    double precision :: normloc
    double precision, external :: ddot

    allocate(a(nvec))
    print *,'GS> ----------------------'
    print *,"GS> Gram-Schmidt algorithm"
    print *,'GS> ----------------------'
    print *,'GS> ',nvec,' vectors to orthogonalize'
    print *,'GS> ',GS%nindep,' vectors are already orthogonalized'
    Vout(:,1:GS%nindep)=Vin(:,1:GS%nindep)
    GS%ndep=0
    i0=GS%nindep
    do i=i0+1,nvec
       Vout(:,GS%nindep+1)=Vin(:,i)
       do k=1,GS%nindep
          ! We compute the projection of Vini(:,i) on V(:,1-nindep)
          a(k)=ddot(m%N,Vout(:,k),1,Vin(:,i),1)
          !print *,'GS > ',i,k,a(k)
          ! then we remove V(:,k) from V(:,nindep+1)
          call daxpy(m%N,-a(k),Vout(:,k),1,Vout(:,GS%nindep+1),1)
       end do
       ! now wre compute the norm of V(:,nindep+1)
       normloc=sqrt(ddot(m%N,Vout(:,GS%nindep+1),1,Vout(:,GS%nindep+1),1))
       !print *,'GS > norm(',i,')=',norm
       if (normloc.le.ETA) then
          GS%ndep=GS%ndep+1 ! V(:,nindep+1) is not linearly inependent
       else
          normloc=1.0/normloc
          call dscal(m%N,normloc,Vout(:,GS%nindep+1),1)
          !              do k=2,icur
          !                 print *,'<U',k-1,'|U',i,'>=',ddot(N,V(:,k-1),1,V(:,icur),1)
          !              end do
          GS%nindep=GS%nindep+1
       end if
    end do
    print *,'GS> ',GS%ndep,' vectors linearly dependant'
    print *,'GS> ',GS%nindep,' vectors linearly independant'
    print *,'GS> Size of the basis from ',nvec,' to ',GS%nindep
    !call check_ortho(Vout,nvec,m)
    !stop
    nvec=GS%nindep
    deallocate(a)
  end subroutine GramSchmidt
  ! ---------------------------------------------
  subroutine check_ortho(P,nvec,m)
    implicit none
    integer :: nvec
    double precision :: P(:,:)
    type(t_mesh)::m

    double precision, parameter :: ETA=1.0e-6
    integer :: i,j,nfail
    double precision :: pscal
    double precision, external :: ddot
    nfail=-nvec
    print *,"--- check_ortho() ---"
    do i=1,nvec
       do j=1,nvec
          pscal=ddot(m%N,P(:,i),1,P(:,j),1)
          write(*,'(F10.2)',advance='no') pscal
          if (pscal.gt.ETA) nfail=nfail+1
       end do
       write(*,*)
    end do
    if (nfail.gt.0) then
       print *,nfail,' fail(s)'
       stop
    end if
  end subroutine check_ortho


  ! ---------------------------------------------
  subroutine init_mesh(m,param)
    implicit none
    type(t_mesh)::m
    type(t_param)::param
    double precision:: Lwidth

    Lwidth=param%box_width
    m%Nx=param%Nx
!    m%Nx=5
    m%Ny=m%Nx
    m%Nz=m%Nx
```

```
    m%N=m%Nx*m%Ny*m%Nz

    m%dx=Lwidth/(m%Nx+1)
    m%dy=Lwidth/(m%Ny+1)
    m%dz=Lwidth/(m%Nz+1)
    m%dv=m%dx*m%dy*m%dz
    !m%dv=1.0

    m%center(1)=Lwidth/2
    m%center(2)=Lwidth/2
    m%center(3)=Lwidth/2

    allocate(m%n_neighbors(m%N))
    allocate(m%list_neighbors(m%N,6)) !
    m%list_neighbors(:,:)=0
    m%n_neighbors(:)=0
    call compute_list_neighbors(m)
  end subroutine init_mesh
  ! --------------------------------------------------
  subroutine free_mesh(m)
    implicit none
    type(t_mesh) :: m
    deallocate(m%n_neighbors)
    deallocate(m%list_neighbors) !
  end subroutine free_mesh
  ! --------------------------------------------------
  subroutine compute_list_neighbors(m)
    implicit none
    type(t_mesh) :: m
    integer::i,j,k,nn
    !integer,allocatable::n_neighbors(:),list_neighbors(:,:)

    do k=1,m%Nz
       do i=1,m%Nx
          do j=1,m%Ny
             nn=j+(i-1)*m%Ny+(k-1)*m%Ny*m%Nx
             if (k>1) then
                m%n_neighbors(nn)=m%n_neighbors(nn)+1
                m%list_neighbors(nn,m%n_neighbors(nn))=nn-m%Nx*m%Ny
             end if
             if (k<m%Nz) then
                m%n_neighbors(nn)=m%n_neighbors(nn)+1
                m%list_neighbors(nn,m%n_neighbors(nn))=nn+m%Nx*m%Ny
             end if
             if (i>1) then
                m%n_neighbors(nn)=m%n_neighbors(nn)+1
                m%list_neighbors(nn,m%n_neighbors(nn))=nn-m%Ny
             end if
             if (i<m%Nx) then
                m%n_neighbors(nn)=m%n_neighbors(nn)+1
                m%list_neighbors(nn,m%n_neighbors(nn))=nn+m%Ny
             end if
             if (j>1) then
```

```
              m%n_neighbors(nn)=m%n_neighbors(nn)+1
              m%list_neighbors(nn,m%n_neighbors(nn))=nn-1
           end if
           if (j<m%Ny) then
              m%n_neighbors(nn)=m%n_neighbors(nn)+1
              m%list_neighbors(nn,m%n_neighbors(nn))=nn+1
           end if
        end do
     end do
  end do

 end subroutine compute_list_neighbors


end program Hbinitio
```

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