

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 1/10

```

#include "numbat_decl.h"

! q_ac : acoustic wave number (q_ac)
! n_modes: desired number of solved acoustic modes
! n_msh_pts: number of nodes in mesh
! n_msh_el: number of (triang) elements in mesh
! n_v_el_material: number of types of material
! v_nd_physindex: ??
! elnd_to_mshpt:
! v_el_material:
! v_nd_xy
! v_eigs_nu: eigen frequencies nu=omega/(2D_PI) for each mode
! femsol_ac:
! poln_fracs:

module calc_ac_impl

  use numbatmod
  use alloc

  use class Stopwatch
  use class MeshRaw
  use class SparseCSC_AC

contains

  subroutine calc_ac_modes_impl(n_modes, q_ac, dimscale_in_m, shift_nu, &
    bdy_cdn, itermx, tol, debug, show_mem_est, &
    symmetry_flag, n_elt_mats, c_tensor, rho, supplied_geo_flag, &
    mesh_file, n_msh_pts, n_msh_el, &
    v_nd_physindex, &
    elnd_to_mshpt, v_el_material, v_nd_xy, &
    v_eigs_nu, femsol_ac, poln_fracs, nberr)

    integer(8), intent(in) :: n_modes

    complex(8), intent(in) :: q_ac
    double precision, intent(in) :: dimscale_in_m
    complex(8), intent(in) :: shift_nu
    integer(8), intent(in) :: bdy_cdn, itermx, debug, show_mem_est
    double precision, intent(in) :: tol
    integer(8), intent(in) :: symmetry_flag, supplied_geo_flag
    integer(8), intent(in) :: n_elt_mats

    complex(8), intent(in) :: c_tensor(6,6,n_elt_mats)
    complex(8), intent(in) :: rho(n_elt_mats)

    character(len=FNAME_LENGTH), intent(in) :: mesh_file
    integer(8), intent(in) :: n_msh_pts, n_msh_el

    integer(8), intent(in) :: v_nd_physindex(n_msh_pts)

    integer(8), intent(inout) :: v_el_material(n_msh_el)
    integer(8), intent(inout) :: elnd_to_mshpt(P2_NODES_PER_EL, n_msh_el)

    double precision, intent(inout) :: v_nd_xy(2,n_msh_pts)

    complex(8), intent(out), target :: v_eigs_nu(n_modes)
    complex(8), intent(out), target :: femsol_ac(3,P2_NODES_PER_EL,n_modes,n_m

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 2/10

```

sh_el)
  complex(8), intent(out) :: poln_fracs(4,n_modes)

  type(NBError) nberr

  ! locals

  type(MeshRawAC) mesh_raw
  type(MeshEntitiesAC) entities
  type(SparseCSC_AC) cscmat

  integer(8) :: errco
  character(len=EMSG_LENGTH) :: emsg

  integer(8) int_max, cmplx_max, int_used, cmplx_used
  integer(8) real_max, real_used, n_ddl
  integer(8) n_dof

  integer(8) :: alloc_stat

  integer(8), dimension(:), allocatable :: a_iwork
  complex(8), dimension(:), allocatable :: b_zwork
  double precision, dimension(:), allocatable :: c_dwork

  !double precision, dimension(:,:), allocatable :: d_dwork
  !complex(8), dimension(:,:), allocatable :: dummy_overlap_L ! not actual
  ly used.

  ! Declare the pointers of the integer(8) super-vector
  integer(8) ip_eq
  integer(8) ip_visited

  ! Declare the pointers of the real super-vector
  integer(8) jp_x, jp_mat2
  integer(8) jp_vect1, jp_vect2, jp_workd, jp_resid, jp_vschur
  integer(8) jp_trav, jp_vp, jp_rhs
  integer(8) jp_eigenmodes_tmp, jp_eigen_pol

  ! Declare the pointers of the real super-vector
  integer(8) kp_mat1_re, kp_mat1_im
  integer(8) kp_rhs_re, kp_rhs_im, kp_lhs_re, kp_lhs_im

  ! Declare the pointers of for sparse matrix storage
  integer(8) ip_col_ptr, ip_row
  integer(8) ip_work, ip_work_sort, ip_work_sort2
  integer(8) nonz, nonz_max, max_row_len

  integer(8) i, j, ip
  integer(8) ui_out, namelength

  !double precision lat_vecs(2,2)
  double precision dim_x, dim_y

  complex(8) shift_omsq
  integer(8) i_base

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 3/10

```

! Variable used by valpr
integer(8) ltrav, n_conv
complex(8) z_beta, z_tmp, z_tmp0
integer(8), dimension(:), allocatable :: iindex
! variable used by UMFPAK

!character*(8) start_date, end_date
!character*(10) start_time, end_time

! Variable used by valpr
integer(8) nvect

! Names and Controls

character(len=FNAME_LENGTH) gmsh_file, log_file, gmsh_file_pos

type(Stopwatch) :: clock_main, clock_spare

integer(8) :: is_em

errco = 0

ui_out = stdout

! nvect = 2*n_modes + n_modes/2 +3
nvect = 3*n_modes + 3

errco= 0
emsg = ""

call mesh_raw%allocate(n_msh_pts, n_msh_el, n_elt_mats, nberr)
RET_ON_NBERR(nberr)

call entities%allocate(n_msh_el, nberr)
RET_ON_NBERR(nberr)

call array_size(n_msh_pts, n_msh_el, n_modes, int_max, cmplx_max, real_max
, &
n_ddl, errco, emsg)
call nberr%set(errco, emsg); RET_ON_NBERR(nberr)

allocate(a_iwork(int_max), STAT=alloc_stat)
call check_alloc(alloc_stat, int_max, "a", -1, nberr);
RET_ON_NBERR(nberr)

allocate(b_zwork(cmplx_max), STAT=alloc_stat)
call check_alloc(alloc_stat, cmplx_max, "b", -1, nberr); RET_ON_NBERR(nber
r)

allocate(c_dwork(real_max), STAT=alloc_stat)
call check_alloc(alloc_stat, real_max, "c", -1, nberr); RET_ON_NBERR(nber
r)

allocate(iindex(n_modes), STAT=alloc_stat)
call check_alloc(alloc_stat, n_modes, "iindex", -1, nberr); RET_ON_NBERR(nb
err)

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 4/10

```

is_em = 0

! clean mesh_format
namelength = len_trim(mesh_file)
gmsh_file = mesh_file(1:namelength-5)///'.msh'
gmsh_file_pos = mesh_file(1:namelength)
log_file = mesh_file(1:namelength-5)///'-AC.log'
if (debug .eq. 1) then
    write(*,*) "mesh_file = ", mesh_file
    write(*,*) "gmsh_file = ", gmsh_file
endif

dim_x = dimscaled_in_m
dim_y = dimscaled_in_m
shift_omsq= (2*D_PI*shift_nu)**2

! pointer to FEM connectivity table
ip_visited= 1
ip_eq = ip_visited+ n_msh_pts
jp_x = 1
!

call clock_main%reset()

if (supplied_geo_flag .eq. 0) then
    call construct_fem_node_tables_ac (mesh_file, dim_x, dim_y, n_msh_el, n
_msh_pts, &
P2_NODES_PER_EL, n_elt_mats, v_nd_xy, v_nd_physindex, v_el_material,
elnd_to_mshpt, errco, emsg)
    call nberr%set(errco, emsg); RET_ON_NBERR(nberr)
endif

! Fills: MeshRaw: v_nd_xy, v_nd_physindex, v_el_material, elnd_to_mshpt
! This knows the position and material of each elt and mesh point but not
their connectedness or edge/face nature

if (supplied_geo_flag .eq. 0) then
    call mesh_raw%construct_node_tables(mesh_file, dimscaled_in_m, nberr);
    RET_ON_NBERR(nberr)
else
    call mesh_raw%load_node_tables_from_py(v_nd_xy, v_nd_physindex, &
v_el_material, elnd_to_mshpt, nberr);
    RET_ON_NBERR(nberr)
endif

!call periodic_lattice_vec (n_msh_pts, v_nd_xy, lat_vecs, debug)

! Determine number of boundary conditions (n_dof) and 2D index array
! a_iwork(ip_eq)
!call bound_cond_AC (bdy_cdn, n_msh_pts, n_dof, v_nd_physindex, a_iwork(ip
_eq))

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 5/10

```

call bound_cond_AC (bdy_cdn, mesh_raw, n_dof, a_iwork(ip_eq))

call cscmat%set_bound_cond(bdy_cdn, mesh_raw, nberr)
RET_ON_NBERR(nberr)

!
! Sparse matrix storage
ip_col_ptr = ip_eq + 3*n_msh_pts

call csr_make_col_ptr_loose_AC (n_msh_el, n_msh_pts, n_dof, P2_NODES_PER_E
L, &
    elnd_to_mshpt, a_iwork(ip_eq), a_iwork(ip_col_ptr), nonz_max)

ip = ip_col_ptr + n_dof + 1
if (ip .gt. int_max) then
    write (emsg,*) "py_calc_modes_AC: ip > int_max: ", &
        ip, int_max, &
        "py_calc_modes_AC: nonz_max = ", nonz_max, &
        "py_calc_modes_AC: increase the size of int_max"
    errco = -3
    return
endif
!
ip_row = ip_col_ptr + n_dof + 1

call csr_length_AC (n_msh_el, n_msh_pts, n_dof, P2_NODES_PER_EL, &
    elnd_to_mshpt, a_iwork(ip_eq), a_iwork(ip_row), a_iwork(ip_col_ptr), no
nz_max, &
    nonz, max_row_len, ip, int_max, debug)

ip_work = ip_row + nonz
ip_work_sort = ip_work + 3*n_msh_pts
ip_work_sort2 = ip_work_sort + max_row_len

! sorting csr ...
call sort_csr (n_dof, nonz, max_row_len, a_iwork(ip_row), &
    a_iwork(ip_col_ptr), &
    !a_iwork(ip_work_sort),
    a_iwork(ip_work))
!a_iwork(ip_work_sort2)

if (debug .eq. 1) then
    write (ui_out,*) "py_calc_modes_AC: nonz_max = ", nonz_max
    write (ui_out,*) "py_calc_modes_AC: nonz = ", nonz
    write (ui_out,*) "py_calc_modes_AC: cmplx_max/nonz = ", &
        dble(cmplx_max)/dble(nonz)
endif

int_used = ip_work_sort2 + max_row_len

if (int_max .lt. int_used) then
    write (emsg,*) "The size of the integer(8) supervector is too small", &
        "integer(8) super-vec: int_max = ", int_max, &
        "integer(8) super-vec: int_used = ", int_used
    errco = -4
    call nberr%set (errco, emsg); RET_ON_NBERR(nberr)

endif

jp_rhs = jp_x + 2*n_msh_pts
! jp_rhs will also be used (in gmsh_post_process) to store a solution

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 6/10

```

jp_mat2 = jp_rhs + max(n_dof, 3*n_msh_pts)
jp_vect1 = jp_mat2 + nonz
jp_vect2 = jp_vect1 + n_dof
jp_workd = jp_vect2 + n_dof
jp_resid = jp_workd + 3*n_dof
jp_eigenum_modes_tmp = jp_resid+3*P2_NODES_PER_EL*n_modes*n_msh_el
! Eigenvectors
jp_vschur = jp_eigenum_modes_tmp + n_modes + 1
jp_eigen_pol = jp_vschur + n_dof*nvect
jp_trav = jp_eigen_pol + n_modes*4

ltrav = 3*nvect*(nvect+2)
jp_vp = jp_trav + ltrav
cmplx_used = jp_vp + n_dof*n_modes

if (cmplx_max .lt. cmplx_used) then
    write (emsg,*) "The size of the complex supervector is too small", &
        "complex super-vec: cmplx_max = ", cmplx_max, &
        "complex super-vec: cmplx_used = ", cmplx_used
    errco = -5
    call nberr%set (errco, emsg); RET_ON_NBERR(nberr)
endif

kp_rhs_re = 1
kp_rhs_im = kp_rhs_re + n_dof
kp_lhs_re = kp_rhs_im + n_dof
kp_lhs_im = kp_lhs_re + n_dof
kp_mat1_re = kp_lhs_im + n_dof
kp_mat1_im = kp_mat1_re + nonz
real_used = kp_mat1_im + nonz

if (real_max .lt. real_used) then
    write (ui_out,*)
    write (ui_out,*) "The size of the real supervector is too small"
    write (ui_out,*) "2*nonz = ", 2*nonz
    write (ui_out,*) "real super-vec: real_max = ", real_max
    write (ui_out,*) "real super-vec: real_used = ", real_used

    write (emsg,*) "The size of the real supervector is too small", &
        "2*nonz = ", 2*nonz, &
        "real super-vec: real_max = ", real_max, &
        "real super-vec: real_used = ", real_used

    errco = -6
    call nberr%set (errco, emsg); RET_ON_NBERR(nberr)
    return
endif

!
! #####
!
! -----
! convert from 1-based to 0-based
! -----
!

do 60 j = 1, n_dof+1
    a_iwork(j+ip_col_ptr-1) = a_iwork(j+ip_col_ptr-1) - 1
continue
do 70 j = 1, nonz
    a_iwork(j+ip_row-1) = a_iwork(j+ip_row-1) - 1

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 7/10

```

70  continue
!
!
! The CSC iindexing, i.e., ip_col_ptr, is 1-based
! (but valpr.f will change the CSC iindexing to 0-based iindexing)
i_base = 0

!##### End FEM PRE-PROCESSING #####
!
write(ui_out,*)
write(ui_out,*) "-----"
! write(ui_out,*) " AC FEM, k_AC : ", real(q_ac), " 1/m"
! write(ui_out,*) "-----"
! write(ui_out,*)

! if (debug .eq. 1) then
! write(ui_out,*) "py_calc_modes_AC: call to asmbly"
! endif
write(ui_out,*) "AC FEM: "

! Assemble the coefficient matrix K and M of the finite element equations

write(ui_out, '(A,A)') " - assembling linear system:"
call clock_spare%reset()

call asmbly_AC (i_base, n_msh_el, n_msh_pts, n_dof, P2_NODES_PER_EL, &
  shift_omsq, q_ac, n_elt_mats, rho, c_tensor, &
  elnd_to_mshpt, v_el_material, a_iwork(ip_eq), &
  v_nd_xy, nonz, a_iwork(ip_row), a_iwork(ip_col_ptr), &
  c_dwork(kp_mat1_re), c_dwork(kp_mat1_im), b_zwork(jp_mat2), a_iwork(ip_
work), &
  symmetry_flag, debug)

write(ui_out, '(A,i9,A)') ' ', n_msh_el, ' mesh elements'
write(ui_out, '(A,i9,A)') ' ', n_msh_pts, ' mesh nodes'
write(ui_out, '(A,i9,A)') ' ', n_dof, ' linear equations'
write(ui_out, '(A,i9,A)') ' ', nonz, ' nonzero elements'
write(ui_out, '(A,f9.3,A)') ' ', nonz/(1.d0*n_dof*n_dof)*100.d0, ' % sparsity'
write(ui_out, '(A,i9,A)') ' ', n_dof*(nvect+6)*16/2**20, ' MB est. working memory'

write(ui_out, '(/(A,A)') ' ', clock_spare%to_string()

write(ui_out, '(/(A)') " - solving linear system: "
write(ui_out, '(/(A)') " solving eigensystem"
call clock_spare%reset()

call valpr_64_AC (i_base, nvect, n_modes, n_dof, itermax, ltrav, &
  tol, nonz, a_iwork(ip_row), a_iwork(ip_col_ptr), c_dwork(kp_mat1_re), &
  c_dwork(kp_mat1_im), b_zwork(jp_mat2), &
  b_zwork(jp_vect1), b_zwork(jp_vect2), b_zwork(jp_workd), b_zwork(jp_res
id), &
  b_zwork(jp_vschor), v_eigs_nu, b_zwork(jp_trav), b_zwork(jp_vp), &
  c_dwork(kp_rhs_re), c_dwork(kp_rhs_im), c_dwork(kp_lhs_re), c_dwork(kp_
lhs_im), n_conv, &
  debug, show_mem_est, errco, emsg)

call nberr%set(errco, emsg); RET_ON_NBERR(nberr)

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 8/10

```

if (n_conv .ne. n_modes) then
  write(emsg, '(A,I5,I5)') &
    "py_calc_modes_AC: convergence problem " // &
    "in valpr_64: n_conv != n_modes ", n_conv, n_modes
  errco = -7
  call nberr%set(errco, emsg); RET_ON_NBERR(nberr)
endif

write(ui_out, '(A,A)') ' ', clock_spare%to_string()

write(ui_out, '(/(A)') " assembling modes"
call clock_spare%reset()

!
do i=1, n_modes
  z_tmp0 = v_eigs_nu(i)
  z_tmp = 1.0d0/z_tmp0+shift_omsq
  z_beta = sqrt(z_tmp) / (2.0d0 * D_PI)
  ! Frequency (z_beta) should always be positive.
  if (dble(z_beta) .lt. 0) z_beta = -z_beta
  v_eigs_nu(i) = z_beta
enddo

!
call z_indexx_AC (n_modes, v_eigs_nu, iindex)
!
! The eigenvectors will be stored in the array femsol_ac
! The eigenmodes and eigenvectors will be renumbered
! using the permutation vector iindex
if (debug .eq. 1) then
  write(ui_out,*) "py_calc_modes_AC: call to array_sol"
endif
call array_sol_AC (n_modes, n_msh_el, n_msh_pts, n_dof, &
  P2_NODES_PER_EL, iindex, elnd_to_mshpt, v_el_material, a_iwork(ip_eq),
  v_nd_xy, &
  v_eigs_nu, b_zwork(jp_eigenmodes_tmp), poln_fracs, b_zwork(jp_vp),
  femsol_ac)

if (debug .eq. 1) then
  write(ui_out,*) "py_calc_modes_AC: array_sol returns call"
endif
!
if (debug .eq. 1) then
  write(ui_out,*) 'iindex = ', (iindex(i), i=1, n_modes)
endif
if (debug .eq. 1) then
  write(ui_out,*)
  ! write(ui_out,*) "lambda, 1/lambda = ", lambda, 1.0d0/lambda
  ! write(ui_out,*) "sqrt(shift_omsq)/(2*D_PI) = ", sqrt(omsq) / (2.0d0
* D_PI)
  do i=1, n_modes
    write(ui_out, "(i4,2(g22.14),2(g18.10))") i, v_eigs_nu(i)
  enddo
endif

!C Save Original solution
! if (plot_modes .eq. 1) then
! dir_name = "AC_fields"
!C call write_sol_AC (n_modes, n_msh_el, P2_NODES_PER_EL, lambda,

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 9/10

```

!C      *      v_eigs_nu, femsol_ac, mesh_file, dir_name)
!C      call write_param (lambda, n_msh_pts, n_msh_el, bdy_cdn,
!C      *      n_modes, nvect, itermax, tol, shift_omsq, lx, ly,
!C      *      mesh_file, n_conv, dir_name)
!      tchar = "AC_fields/All_plots_png_abs2_eE.geo"
!      open (unit=34,file=tchar)
!      do i=1,n_modes
!      call gmsh_post_process_AC (i, n_modes, n_msh_el,
!      *      n_msh_pts, P2_NODES_PER_EL, elnd_to_mshpt, v_el_material,
!      *      v_nd_xy, v_eigs_nu, femsol_ac, b_zwork(jp_rhs), a_iwork(ip_vi
site),
!      *      gmsh_file_pos, dir_name, dimscale_in_m, debug)
!      enddo
!      close (unit=34)
!      endif
!C
!
!##### End Calculations #####
!
!      call date_and_time ( end_date, end_time )
!      call cpu_time(time2)
!
!      if (debug .eq. 1) then
!      write(ui_out,*)
!      write(ui_out,*) 'Total CPU time (sec.) = ', (time2-time1)
!
!      open (unit=26,file=log_file)
!      write(26,*)
!      write(26,*) "Date and time formats = ccyyymmdd ; hhmmss.sss"
!      write(26,*) "Start date and time   = ", start_date, &
!      " ; ", start_time
!      write(26,*) "End date and time     = ", end_date, &
!      " ; ", end_time
!      write(26,*) "Total CPU time (sec.) = ", (time2-time1)
!      write(26,*)
!      write(26,*) "q_ac = ", q_ac
!      write(26,*) "shift_omsq= ", shift_omsq
!      write(26,*)
!      write(26,*) "n_msh_pts, n_msh_el, P2_NODES_PER_EL = ", n_msh_pts, &
!      n_msh_el, P2_NODES_PER_EL
!      write(26,*) "n_dof, bdy_cdn = ", n_dof, bdy_cdn
!      write(26,*) " lat_vecs: = "
!      write(26,"(2(f18.10))") lat_vecs
!      write(26,*) "mesh_file = ", mesh_file
!      write(26,*) "gmsh_file = ", gmsh_file
!      write(26,*) "log_file = ", log_file
!      close(26)
!
!      write(ui_out,*) "      .      ."
!      write(ui_out,*) "      .      ."
!      write(ui_out,*) "      .      . (d=",dimscale_in_m,") "
!      write(ui_out,*) " and we're done!"
!      endif

write(ui_out,'(A,A)') '      ', clock_spare%to_string()
write(ui_out,*) "-----"
write(ui_out,*)
!
deallocate(a_iwork, b_zwork, c_dwork, iindex)

end subroutine calc_ac_modes_impl

```

Jan 22, 2025 15:49

py_calc_modes_ac.f90

Page 10/10

```

end module calc_ac_impl

```