

# User Manual of the TASK/FP Code

## Contents

## 1 Structure

### 1.1 Environment routines

- **fpcomm.f90**: Definition of variable module, allocation of arrays
  - **Module fpcomm\_parm**: Definition of constants and input parameters including
    - \* bpsd\_kinds
    - \* bpsd\_constants
    - \* commpi
    - \* plcomm
    - \* obcomm\_parm
  - **Module fpcomm**: Definition of common variables
  - **Subroutine fp\_allocate**: Allocation of common arrays
  - **Subroutine fp\_deallocate**: Deallocation of common arrays
  - **Subroutine fp\_allocate\_ntg1**: Allocation of time history ntg1 array
  - **Subroutine fp\_deallocate\_ntg1**: Deallocation of time history ntg1 array
  - **Subroutine fp\_adjust\_ntg1**: Adjust (save, deallocate, allocate larger, recover) time history ntg1 array
  - **Subroutine fp\_allocate\_ntg2**: Allocation of profile time history ntg2 array
  - **Subroutine fp\_deallocate\_ntg2**: Deallocation of profile time history ntg2 array
  - **Subroutine fp\_adjust\_ntg2**: Adjust (save, deallocate, allocate larger, recover) profile time history ntg2 array
- **fpmain.f90**: Main routine
  - **Program fp**
    - \* Initialization of MPI and graphics
    - \* Initialization of input parameters of module, pl, eq, and fp
    - \* Read input namelist file fpparm
    - \* Start menu input loop fpmenu
    - \* Termination of graphics and MPI
- **fpinit.f90**: **Module fpinit**: Initialization of input parameters
  - **Subroutine fp\_init**: Set default values of input parameters
- **fpmenu.f90**: **Module fpmenu**: Process control
  - **Subroutine fp\_menu**: menu command input and execute
    - \* P or with =: namelist read of input parameters
    - \* V: view all input parameters

- \* R: start new calculation (set initial condition and go)
  - \* C: continue previous calculation (just go)
  - \* G: graphic output of calculated results
  - \* F: file output of calculated results
  - \* S: save present status of calculation into a file
  - \* L: load a file to continue previous calculation
  - \* W: print out interesting quantities
  - \* Y: debug output [temporal]
  - \* Z: debug output [transport coefficients]
  - \* Q: quit menu input and stop
- **fpparm.f90**: **Module fpparm**: Read and check input parameters
    - **Subroutine fp\_parm**: analyze parameter input
      - \* read one line from standard input and analyze command or namelist
      - \* read namelist input from a file
      - \* read one phrase and analyze as a namelist
    - **Subroutine fp\_nlin**: namelist input slave routine
    - **Subroutine fp\_plst**: input parameter list slave routine
    - **Subroutine fp\_check**: input parameter check
    - **Subroutine fp\_broadcast**: Broadcast input parameters
    - **Subroutine fp\_view**: Show input parameters

## 1.2 Execution routines

- **fpprep.f90**: **Module fpprep**: Preparation of run (mesh, initial profile, initialization)
  - **Subroutine fp\_mesh**: create mesh quantities
    - \* set pmax
    - \* read EQ data (RKAP=1.0 should be removed)
    - \* set radial mesh
    - \* read WR data
    - \* read WM data
    - \* set approximate poloidal magnetic field (exact poloidal magnetic field should be used)
    - \* set momentum space mesh
    - \* set element volume in real space
    - \* set bounce-average parameters
  - **Subroutine FPCINI**: clear friction and diffusion coefficients
  - **Subroutine fp\_comm\_setup**: check partitions and setup shadow and communicators
  - **Subroutine fp\_set\_nsa\_nsb**: set table on nsa and nsb
  - **Subroutine FNSP\_INIT**: initialize distribution functions FNSP and delta f
  - **Subroutine FNSP\_INIT\_EDGE**: initialize edge distribution functions FS1, FS2
  - **Subroutine fp\_set\_normalize\_param**: set normalized density, temperature and other quantities

- **Subroutine** `Coulomb_log`: calculate Coulomb logarithm
- **Subroutine** `fp_continue`: setup for continuation
- **Subroutine** `fp_set_initial_value_from_f`: record initial values
- **Subroutine** `fp_prep`:
  - \* initialize time counter
  - \* allocate variables
  - \* setup matrix parameters for MPI
  - \* setup particle species table (`fp_set_nsa_nsa`)
  - \* create mesh (`fp_mesh`)
  - \* initialize diffusion coefficients (`FPCINI`)
  - \* set parameters (`fp_set_normalize_param`)
  - \* initialize distribution functions (`FNSP_INIT`, `FNSP_INIT_EDGE`)
  - \* set background distribution functions (`update_fnsb`)
  - \* read FIT3D results for NBI (`READ_FIT3D`, `SV_WEIGHT_R`)
  - \* set parallel electric field
  - \* setup for Legendre expansion and fusion reaction rate (`NF_*`)
  - \* record initial values (`fp_set_initial_value_from_f`)
- `fpbounce.f90`: Preparation of bounce parameters
- `fploop.f90`: Time loop for execution
- `fpexec.f90`: Execution of one time step

### 1.3 Calculation of coefficients of equations

- `fpcoef.f90`: Calculation of various coefficients
- `fpcalc.f90`: Calculation of collisional term (linear operator)
- `fpcalcn.f90`: Calculation of collisional term (nonlinear operator)
- `fpcalcnr.f90`: Calculation of collisional term (relativistic nonlinear operator)
- `fpcale.f90`: Calculation of static electric field term
- `fpcalr.f90`: Calculation of radial diffusion term
- `fpcalw.f90`: Calculation of quasi-linear term (given wave field)
- `fpcalwm.f90`: Calculation of quasi-linear term (using wm results)
- `fpcalwr.f90`: Calculation of quasi-linear term (using wr results)
- `fpcdbm.f90`: Calculation of CDBM radial diffusion coefficients
- `fpnfrr.f90`: Calculation of fusion reaction term (isotropic distribution)
- `fpnflg.f90`: Calculation of fusion reaction term (anisotropic distribution)
- `fpdisrupt.f90`: Calculation of disruption-related terms

#### 1.4 Calculation of transport coefficients (by Ota)

- `fpcaldeff.f90`: Effective particle diffusion coefficients
- `fpcalchieff.f90`: Effective thermal diffusion coefficients
- `fpcaltp.f90`: Particle confinement time,  $\tau_P$
- `fpcalte.f90`: Energy confinement time,  $\tau_E$
- `fpchecknc.f90`: Radial diffusion coefficients (neoclassical diffusion)

#### 1.5 File IO routines

- `fpfile.f90`: Save and load restart data
- `fpfout.f90`: File output of graphic data
- `fpoutdata.f90`: File output of intermediate data (by Ota)
- `fpread.f90`: Read FIT3D data from file
- `fpreadeg.f90`: Read Experimental data from file (by Nuga)
- `fpsave.f90`: File output of various data (by Nuga)
- `fpwmin.f90`: File input of full-wave analysis (wm) results
- `fpwrin.f90`: File input of ray/beam tracing analysis (wr) results
- `fpwrite.f90`: File output of trcoef data (by Ota)

#### 1.6 Graphic routines

- `fpgout.f90`: Graphic output for gsaf
- `fpcont.f90`: Graphic subroutines

#### 1.7 Library routines

- `fpmpi.f90`: MPI interface for fp
- `fpsub.f90`: Subroutine library (FPMXWL, FPNEWTON)

#### 1.8 Orbit-averaging routines (by Ota)

- `fowcomm.f90`: Definition of fow variables and allocation
  - **Module** `fowcomm`: define quantities related to orbit-averaging
  - **Subroutine** `fow_allocate`: allocate adjustable arrays
  - **Subroutine** `fow_deallocate`: deallocate adjustable arrays
- `fowprep.f90`: **Module** `fowprep`: Preparation of fow, initialization of variables
  - **Subroutine** `search_pinch_orbit`: calculate pinch orbit
  - **Subroutine** `calculate_jacobian`: calculation of jacobians
- `foworbit.f90`: **Module** `foworbit`: Interface to ob

- **Subroutine** `fow_set_obparm`
    - \* `ob_init`, `ob_parm`, `ob_prep`, `ob_allocate`, and spline `psim`, `Fpsi`, `B`, `dradpsi`
  - **Subroutine** `fow_orbit`
    - \* calculated orbits
  - **Subroutine** `fow_cal_local_COMs`
    - \* calculate `thetaml`, `rhoml`, `tau_loss`
  - **Subroutine** `construct_orbit`
    - \* call `ob_calc` to calculate ob structure
  - **Subroutine** `construct_orbit_zero`
    - \* set zero into ob structure
  - **Subroutine** `save_orbit`
    - \* save orbit data into file
  - **Subroutine** `load_orbit`
    - \* load orbit data from file
  - **Subroutine** `quantities_at_Bminimum`
    - \* calculate quantities at `B_min`
  - **Subroutine** `mean_ra_quantities`
    - \* calculate quantities at average radius
- **`fowclassify.f90`: Module `fowclasify`:** Orbit classification and data output to file
    - **Subroutine** `output_orbit_cllasify`:
      - \* `prep_orbit_classify`
      - \* `pinch_orbit`
      - \* `D_orbit(beta_D)`
      - \* `stagnation_orbit(beta_stag)`
      - \* `stagnation_type(xi_Xtype_boundary_ion)`
      - \* output to file `dat/*_obclass.txt`
    - **Subroutine** `prep_orbit_classify`: calculate `theta_m` and `xi`
    - **Subroutine** `pinch_orbit`: calculate all pinch points
    - **Subroutine** `get_pinch_point`: calculate momentum of one pinch orbit
    - **Subroutine** `D_orbit`: calculate maximum momentum of trapped particle
    - **Subroutine** `stagnation_orbit`: calculate maximum momentum of not-forbidden orbit
    - **Subroutine** `stagnation_type`:
  - **`fowdistribution.f90`:** Distribution conversion and integrated quantities
    - **Subroutine** `fI_Maxwellian`: calculate Maxwellian distribution
    - **Subroutine** `convert_fI_to_fu`: convert `f(I)` to `f(local)`
    - **Subroutine** `moment_0th_order_COM`: calculate 0th order momentum from `f(I)`
    - **Subroutine** `moment_2nd_order_COM`: calculate 2nd order momentum from `f(I)`
    - **Subroutine** `particle_flux`: calculate total particle flux
    - **Subroutine** `particle_flux_element`: calculate particle flux from each component

- **Subroutine** `total_N`: calculate total density
- **Subroutine** `effective_diffusion_coef`: calculate particle diffusion coefficient from particle flux and density gradient
- `fowloop.f90`: `fmodfowloop`: Time loop for execution
  - **Subroutine** `fow_loop`:
    - \* `fl_Maxwellian`: calculate initial distribution function
    - \* `fow_coef`: calculate transport coefficients
    - \* `fow_calculate_source`: calculate source
    - \* `loop`: call `fow_exec`, update coef
    - \* calculate density and temperature
    - \* output data
  - **Subroutine** `update_bulk_temperature`: calculate temperature
  - **Subroutine** `output_data`: output data to file `dat/*.txt`
- `fowexec.f90`: **Module** `fowexec`: Execution of one time step
  - **Subroutine** `fow_exec`: Execution of one time step
    - \* `mtx_setup`: initialization of matrix solver
    - \* `fowweight`: setup weight array
    - \* `SET_FM_NMA`: setup index array
    - \* `fowsetm`: calculate matrix coefficients in a row
    - \* `IBC_pinch`, `IBC_X_stagnation`, `IBC_O_stagnation`: set internal boundary conditions
    - \* `mtx_set_matrix`, `mtx_set_vector`, `mtx_set_source`: set matrix coefficients, initial solution vector, and right-hand-side vector
    - \* `mtx_solve`, `mtx_get_vector`: solve matrix equation and obtain solution vector
    - \* `shadow_comm_np`, `shadow_comm_nr`: gather solution vector
  - **Subroutine** `SET_FM_NMA`: setup index array
  - **Subroutine** `fowweight`: setup weight array
  - **Function** `fowweigh`: elementary weight function
  - **Subroutine** `fowsetm`: calculate matrix coefficients in a row
  - **Function** `Dfow`: matrix coefficients
  - **Function** `w`: weighting
  - **Function** `check_external_boundary`: check within external boundary
  - **Function** `get_nma`: calculate matrix position
  - **Subroutine** `IBC_pinch`: set pinch boundary condition
  - **Subroutine** `IBC_X_stagnation`: set X stagnation boundary condition
  - **Subroutine** `IBC_O_stagnation`: set O stagnation boundary condition
  - **Function** `f_grid`: evaluate weight on boundary grid point
  - **Function** `nma_boundary`: check `nth`, `np`, `nr` within range (update the evaluation)
- `fowcoef.f90`: **Module** `hfowcccoef`: Calculation of various coefficients
  - **Subroutine** `fow_coef`:

- \* allocate arrays and initialize
  - \* `convert_fI_to_fu`: set local distribution function
  - \* `fp_calc`: calculate local coefficients
  - \* `bounce_average`: bounce average local coefficients
- Subroutine `bounce_average`: bounce average local coefficients
- Subroutine `transformation_matrix`: calculation of transformation matrix
- Subroutine `make_UDxy`: calculation diffusion coefficients in U frame
- Subroutine `interpolate_D_unlessZero`: calculate interpolation coefficients
- `fowsource.f90`: Module `fowsource`: Calculation of source terms
  - Subroutine `fow_calculate_source`:
    - \* `beam_source`: calculate beam source
    - \* set `sppb`
  - Subroutine `beam_source`: calculate and normalize beam source
  - Function `construct_beam`: evaluate `construct_beam`
- `fowlib.f90`: Module `fowlib`: Library for fow
  - Subroutine `solve_quadratic_equation`: quadratic equation solver
  - Subroutine `first_order_derivative`: evaluate first-order derivative
  - Subroutine `second_order_derivative`: evaluate second-order derivative
  - Subroutine `gauss_jordan`: matrix solver
  - Subroutine `fow_cal_spl`: 1D spline for fow
  - Subroutine `fow_cal_spl2D`: 2D spline for fow