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# Data Structures and Code Interfaces of BPSD

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BPSD: Data Exchange Interface
Summary and thoughts

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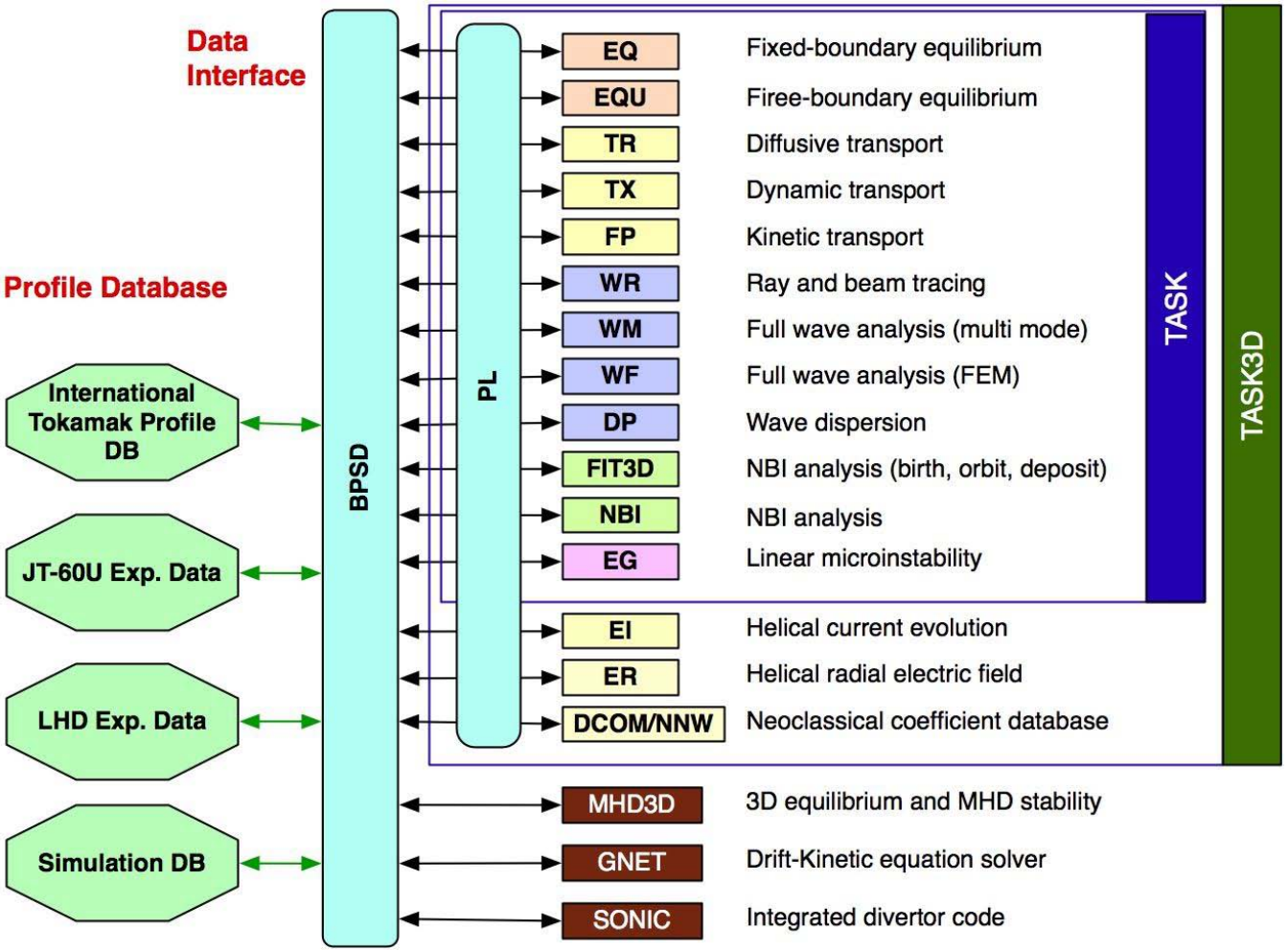
# Structure of TASK, TASK3D, and associated codes

- **BPSI**: Burning Plasma Simulation Initiative (Universities, NIFS, JAEA)
  - **TASK**: Integrated code for tokamak
  - **TASK3D**: Integrated code for 3D configuration (helical, tokamak)



# Component Collaboration

- **Role of Component Interface**
  - **Data exchange between components**: **BPSD**
    - **Standard dataset**: Specify set of data
    - **Specification of data exchange interface**: initialize, set, get
      **Specification of file i/o interface**: save, load
  - **Execution control**: **BPSX**
    - **Specification of execution control interface**:
      initialize, setup, exec, visualize, terminate
    - **Uniform user interface**: parameter input, graphic output
- **Role of data exchange interface: TASK/PL**
  - **Keep present status of plasma and device**
  - **Store history of plasma**
  - **Interface to experimental data base**

# Policies of BPSD

- **Minimum and Sufficient Dataset**
  - **To minimize the data to be exchanged**
  - **Mainly profile data**
  - **Routines to calculate global integrated quantities**
    - separately provided
- **Minimum Arguments in Interfaces**
  - **To maximize flexibility**
  - **Use derived data type or struct**
  - **Only one dataset in the arguments of an interface**
- **Minimum Kinds of Interfaces**
  - **To make modular programming easier**
  - **Use function overloading**
- **Language**: F90/95

# Data Exchange Interface: BPSD

- **Standard dataset**: Specify data to be stored and exchanged
  - **Data structure**: Derived type (Fortran95): structured type

e.g.

| | |
|---|---|
| time | `plasmaf%time` |
| number of grid | `plasmaf%nrmax` |
| number of species | `plasmaf%nsamax` |
| normalized radius | `plasmaf%rho(nr)` |
| Species specifier | `plasmaf%ns(nsa)` |
| plasma density | `plasmaf%data(nr,nsa)%density` |
| plasma temperature | `plasmaf%data(nr,nsa)%temperature` |

- **Specification of API**:
  - **Program interface**

e.g.

| | |
|---|---|
| **Set data** | `bpsd_set_data(plasmaf,ierr)` |
| **Get data** | `bpsd_get_data(plasmaf,ierr)` |
| **Save data to file** | `bpsd_save(ierr)` |
| **Load data from file** | `bpsd_load(ierr)` |

  - **BPSD data file** (bpsddata): Binary file of all existing bpsd data

# BPSD: Standard dataset

- **Internal dataset**: internal use, easier data handling
  - **bpsd_shotx_type**: text data including shotID
  - **bpsd_data0Dx_type**: no profile
  - **bpsd_data1Dx_type**: 1D profile ($\rho$: normalized radius)
  - **bpsd_data2Dx_type**: 2D profile ($\rho$, $\chi$: poloidal angle)
  - **bpsd_data3Dx_type**: 3D profile ($\rho$, $\chi$, $\zeta$: toroidal angle)
- **Standard dataset**: external use, data exchange
  - **User defined dataset**
    - **bpsd_data0D_type, bpsd_data1D_type, bpsd_data2D_type, bpsd_data3D_type**
  - **Predefined dataset**
    - Without dataName: **bpsd_device_type, bpsd_equ1D_type, etc.**
    - With dataName: **bpsd_trmatrix_type**: neoclassical, turbulence, ...
      **bpsd_trsource_type**: $P_{\mathrm{EC}}$, $P_{\mathrm{NB}}$, $S_{\mathrm{NB}}$, ...

# Example of internal dataset structure: data1Dx

```
type bpsd_data1Dx_type
   integer :: status = 0! 0:unalloc 1:undef 2:assigned
                        ! 3:sp-alloc 4:splined
   integer :: nrmax     ! Number of radial points
   integer :: ndmax     ! Number of data
   integer :: idum      ! Dummy
   real(rkind) :: time
   real(rkind), dimension(:), pointer :: rho
   real(rkind), dimension(:,:), pointer :: data
   real(rkind), dimension(:,:,:), pointer :: spline
   character(len=32) :: dataName
   character(len=8)  :: created_date
   character(len=10) :: created_time
   character(len=5)  :: created_timezone
   character(len=9)  :: dummy
   character(len=32), dimension(:), pointer :: kid   ! item name
   character(len=32), dimension(:), pointer :: kunit ! unit of item
end type bpsd_data1Dx_type
```

# BPSD Standard Dataset

| Category | Name | EQ | TR | TX | FP | WR | WM | DP |
|---|---|---|---|---|---|---|---|---|
| Shot data | **bpsd_shot_type** | – | – | – | – | – | – | – |
| Device data | **bpsd_device_type** | in | in | in | in | | | |
| 1D equilibrium data | **bpsd_equ1D_type** | out | in | in | in | | | |
| 2D equilibrium data | **bpsd_equ2D_type** | out | | | in | in | in | in |
| 1D metric data | **bpsd_metric1D_type** | out | in | in | in | | | |
| 2D metric data | **bpsd_metric2D_type** | out | | | in | in | in | in |
| Plasma species data | **bpsd_species_type** | in | in | in | in | | | in |
| Fluid plasma data | **bpsd_plasmaf_type** | in | out | out | i/o | | | in |
| Kinetic plasma data | **bpsd_plasmak_type** | | | | out | | | in |
| Transport matrix data | **bpsd_trmatrix_type** | | i/o | | | | | |
| Transport source data | **bpsd_trsource_type** | | i/o | i/o | i/o | out | out | |
| Dielectric tensor data | **bpsd_dielectric_type** | | | | | in | in | out |
| Full wave field data | **bpsd_wavef_type** | | | | in | out | | |
| Ray tracing field data | **bpsd_waver_type** | | | | in | | out | |
| Beam tracing field data | **bpsd_waveb_type** | | | | in | | out | |
| User defined data | **bpsd_0/1/2ddata_type** | – | – | – | – | – | – | – |

# Defined Dataset (1)

**bpsd_shot_type**

| | | | |
|---|---|---|---|
| DeviceID | | | text |
| ShotID | | | number |
| ModelID | | | number |

**bpsd_device_type**

| | | | |
|---|---|---|---|
| rr | $R$ | m | Geometrical major radius |
| zz | $Z$ | m | Geometrical vertical position |
| ra | $a$ | m | Geometrical minor radius |
| rb | $b$ | m | Wall radius |
| bb | $B$ | T | Vacuum toroidal mag. field |
| ip | $I_{\mathrm{p}}$ | A | Typical plasma current |
| elip | $\kappa$ | | Elongation at boundary |
| trig | $\delta$ | | Triangularity at boundary |

**bpsd_species_type** $n_s$: Particle species ID

| | | |
|---|---|---|
| pa | $A(n_s)$ | Mass number |
| pz | $Z(n_s)$ | Charge number |
| pz0 | $Z_0(n_s)$ | Atomic number |

# Defined Dataset (2)

**bpsd_equ1D_data** ($\rho$: Normalized radius: $\sqrt{\psi_t/\psi_t(a)}$)

| | | | |
|---|---|---|---|
| psit | $\psi_t(\rho)$ | $\mathrm{Tm}^2$ | Toroidal magnetic flux |
| psip | $\psi_p(\rho)$ | $\mathrm{Tm}^2$ | Poloidal magnetic flux |
| ppp | $p(\rho)$ | MPa | Plasma pressure |
| piq | $q(\rho)$ | | Inverse of safety factor |
| pip | $I_t(\rho)$ | Tm | Poloidal current: $2\pi B_\phi R/\mu_0$ |
| pit | $I_p(\rho)$ | Tm | Toroidal current: $2\pi B_\chi r/\mu_0$ |

**bpsd_equ2D_data**

| | | | |
|---|---|---|---|
| psi | $\psi_p(R,Z)$ | $\mathrm{Tm}^2$ | 2D poloidal magnetic flux |

**bpsd_equ3D_data**

| | | | |
|---|---|---|---|
| psi | $\psi_p(R,Z,\phi)$ | $\mathrm{Tm}^2$ | 3D poloidal magnetic flux |

**bpsd_metric1D_data**: $V'(\rho), \langle\nabla V\rangle(\rho), \cdots$

**bpsd_metric2D_data**: $g_{ij}, \cdots$

**bpsd_metric3D_data**: $g_{ij}, \cdots$

# Defined Dataset (3)

## bpsd_plasmaf_data

| | | | |
|---|---|---|---|
| pn | $n_s(\rho)$ | $\mathrm{m}^3$ | Number density |
| pt | $T_s(\rho)$ | eV | Temperature |
| ptpr | $T_{s\|\|}(\rho)$ | eV | Temperature |
| ptpp | $T_{s\perp}(\rho)$ | eV | Temperature |
| pu | $u_{s\phi}(\rho)$ | m/s | Toroidal rotation velocity |
| qinv | $1/q(\rho)$ | | Inverse of safety factor |

## bpsd_plasmak_data

| | | |
|---|---|---|
| fp | $f(p, \theta_p, \rho)$ | momentum dist. fn at $\chi = 0$ |

## bpsd_trmatrix_data

| | | |
|---|---|---|
| trd | $D(i, j, \rho)$ | Diffusion matrix |
| tru | $u(i, \rho)$ | Flow vector |

## bpsd_trsource_data

| | | |
|---|---|---|
| trs | $S(i, \rho)$ | Source vector |

# Defined Dataset (4)

**bpsd_dielectric_data**

| | | | |
|---|---|---|---|
| ceps | $\overleftrightarrow{\epsilon}(\rho,\chi,\zeta)$ | | Local dielectric tensor |

**bpsd_wavef_data**

| | | | |
|---|---|---|---|
| ce | $\boldsymbol{E}(\rho,\chi,\zeta)$ | $\mathrm{V/m}$ | Complex wave electric field |

**bpsd_waver_data**

| | | | |
|---|---|---|---|
| rray | $R(\ell)$ | $\mathrm{m}$ | $R$ of ray at length $\ell$ |
| zray | $Z(\ell)$ | $\mathrm{m}$ | $Z$ of ray at length $\ell$ |
| phiray | $\phi(\ell)$ | $\mathrm{rad}$ | $\phi$ of ray at length $\ell$ |
| ceray | $\boldsymbol{E}(\ell)$ | $\mathrm{V/m}$ | Wave electric field at length $\ell$ |
| pwray | $\boldsymbol{P}(\ell)$ | $\mathrm{W}$ | Wave power at length $\ell$ |

**bpsd_waveb_data**

| | | | |
|---|---|---|---|
| dray | $\boldsymbol{d}(\ell)$ | $\mathrm{m}$ | Beam radius at length $\ell$ |
| vrau | $\boldsymbol{v}(\ell)$ | $1/\mathrm{m}$ | Beam curvature at length $\ell$ |

# Example of data structure: plasmaf

```
type bpsd_plasmaf_data
   real(kind=rkind) :: pn     ! Number density [m^-3]
   real(kind=rkind) :: pt     ! Temperature [eV]
   real(kind=rkind) :: ptpr   ! Parallel temperature [eV]
   real(kind=rkind) :: ptpp   ! Perpendicular temperature [eV]
   real(kind=rkind) :: pu     ! Parallel flow velocity [m/s]
end type bpsd_plasmaf_data

type bpsd_plasmaf_type
   real(kind=rkind) :: time
   integer :: nrmax      ! Number of radial points
   integer :: nsamax     ! Number of particle species
   integer, dimension(:) :: ns_nsa  ! Species specifier
   real(kind=rkind), dimension(:), allocatable :: rho  ! norm. radius
   real(kind=rkind), dimension(:), allocatable :: qinv ! 1/q
   type(bpsd_plasmaf_data), dimension(:,:), allocatable :: data
end type bpsd_plasmaf_type
```

# BPSD Code Interface

- **bpsd_set_data(data,ierr)**:
  - **Copy data into internal dataset**
- **bpsd_get_data(data,ierr)**:
  - **Copy of interpolate data fram internal dataset**
  - If `nrmax=0`, copy data; otherwise interpolate for given mesh.
- **bpsd_save(ierr)**:
  - **Save all BPSD data into a file**
  - Name of the file is optional.
- **bpsd_load(ierr)**:
  - **Load all BPSD data from a file**
  - Name of the file is optional.
- **Interfaces for history archivng are under consideration.**

# Examples of sequence in a component

- **TR_EXEC(dt)**: Transport time evolution

```
call bpsd_get_data(plasmaf,ierr)
call bpsd_get_data(metric1D,ierr)
local data <- plasmaf,metric1D
advance time step dt
plasmaf <- local data
call bpsd_set_data(plasmaf,ierr)
```

- **EQ_CALC**: Equilibrium calculation

```
call bpsd_get_data(plasmaf,ierr)
local data <- plasmaf
calculate equilibrium
update plasmaf
call bpsd_set_data(plasmaf,ierr)
equ1D,metric1D <- local data
call bpsd_set_data(equ1D,ierr)
call bpsd_set_data(metric1D,ierr)
```

# Several Approaches on Workflow

- **Monolithic code approach**: original approach
  - **Memory-based data exchange**
  - **Template**:
    ```
    call bpsd_get_data
    calculation
    call bpsd_set_data
    ```
- **Command approach**: for script and workflow
  - **File-based data exchange**
  - **Template**:
    ```
    call bpsd_load ⟵ bpsddata
    call bpsd_get_data
    calculation
    call bpsd_set_data
    call bpsd_save ⟶ bpsddata
    ```
- **Pre- and post- process approach**: no modification of the code
  - **pre-process**: bpsddata $\Longrightarrow$ input file
  - **post-process**: output file $\Longrightarrow$ bpsddata

# Summary

- For integrated modeling of toroidal plasmas, **platform for data exchange and execution control** is necessary.
- We have been developing **data exchange interface, BPSD**, and implemented in the TASK code.
- Our policy is simple dataset, simple interface, and sufficient flexibility.
- There are several approaches for **workflow**. We are developing
  - **monolithic approach** (memory-based data exchange)
  - **command approach** (file-based data exchange)
  - **pre- and post-process approach** and
  - **MPMD approach** (master-slave using MPI2).
- We have started the discussion on **the data interface for peripheral plasma modeling and atomic data**.

# Thoughts on Future Development

- Dataset specification for **3D configuration** will be completed soon.
- **BPSD data viewer** for monitoring is now under development.
- **Data conversion** between integer mesh and half-integer mesh is troublesome.
- **Data interface between BPSD and IMAS** will be developed, if not incompatible.
- We are watching the IMAS decision on **workflow**
- **Web page**
  - TASK: http://bpsi.nucleng.kyoto-u.ac.jp/task/
  - BPSD: http://bpsi.nucleng.kyoto-u.ac.jp/bpsd/
- **English specification of BPSD** will be uploaded by tomorrow morning.