HDF5 Fortran Interface

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Goal

- Provide an overview of HDF5 Fortran library and how to use it
  - Fortran vs. C storage order
  - HDF5 Fortran APIs
  - HDF5 F2003 programming model
  - Fortran language types vs. HDF5 datatypes

Fortran vs. C Storage Order

C vs. Fortran Storage Order

`h5_rdwt.f90` in `Demo-1` directory writes 2-dim array (4,6)

1	2	3	4	5	6
7	8	9	10	11	12
13	14	15	16	17	18
19	20	21	22	23	24

C vs. Fortran Storage Order (cont'd)

```
$ h5dump file.h5
HDF5 "file.h5" {
GROUP "/" {
   DATASET "A" {
      DATATYPE  H5T_STD_I32LE
      DATASPACE  SIMPLE { ( 6, 4 ) / ( 6, 4 ) }
      DATA {
      (0,0): 1, 7, 13, 19,
      (1,0): 2, 8, 14, 20,
      (2,0): 3, 9, 15, 21,
      (3,0): 4, 10, 16, 22,
      (4,0): 5, 11, 17, 23,
      (5,0): 6, 12, 18, 24
  ...
}
```

1	2	3	4	5	6
7	8	9	10	11	12
13	14	15	16	17	18
19	20	21	22	23	24

h5dump shows transpose data !

C vs. Fortran Storage Order (cont'd)

- HDF5 C library never touches applications' buffer
- Data will be stored as in the application buffer
  - Column order (Fortran)
  - Row order (C)
- HDF5 command-line tools are C tools and display data by row
  - When a C application reads data stored from a Fortran program, the data will appear to be transposed

C vs. Fortran Storage Order

Fastest changing dimension

Fortran storage is by column

1	2	3	4	5	6
7	8	9	10	11	12
13	14	15	16	17	18
19	20	21	22	23	24

C storage is by row

1	7	13	19
2	8	14	20
3	9	15	21
4	10	16	22
5	11	17	23
6	12	18	24

Fastest changing dimension

1	7	13	19	3	9	..	..	23	6	12	18	24

4 elements 4 elements 4 elements

Exercise 1

Example C vs. Fortran

- In EX-1 directory:
  - Run C example h5ex_d_rdwr.c

```
% h5cc h5ex_d_rdwr.c
% ./a.out
```

  - Copy the file h5ex_d_rdwr.h5

```
% cp h5ex_d_rdwr.h5 h5ex_d_rdwr.h5-C
```

  - Run Fortran example h5ex_d_rdwr.f90

```
% h5fc h5ex_d_rdwr.f90
% ./a.out
```

  - Use h5dump to compare output

```
% h5dump h5ex_d_rdwr.h5-C
% h5dump h5ex_d_rdwr.h5
```

FORTRAN APIs

Fortran Examples

- Where to find examples?

Documentation

https://portal.hdfgroup.org/display/HDF5/Examples+by+API

Bitbucket

https://bitbucket.hdfgroup.org/projects/HDFFV/repos/hdf5-examples/browse

Installed code

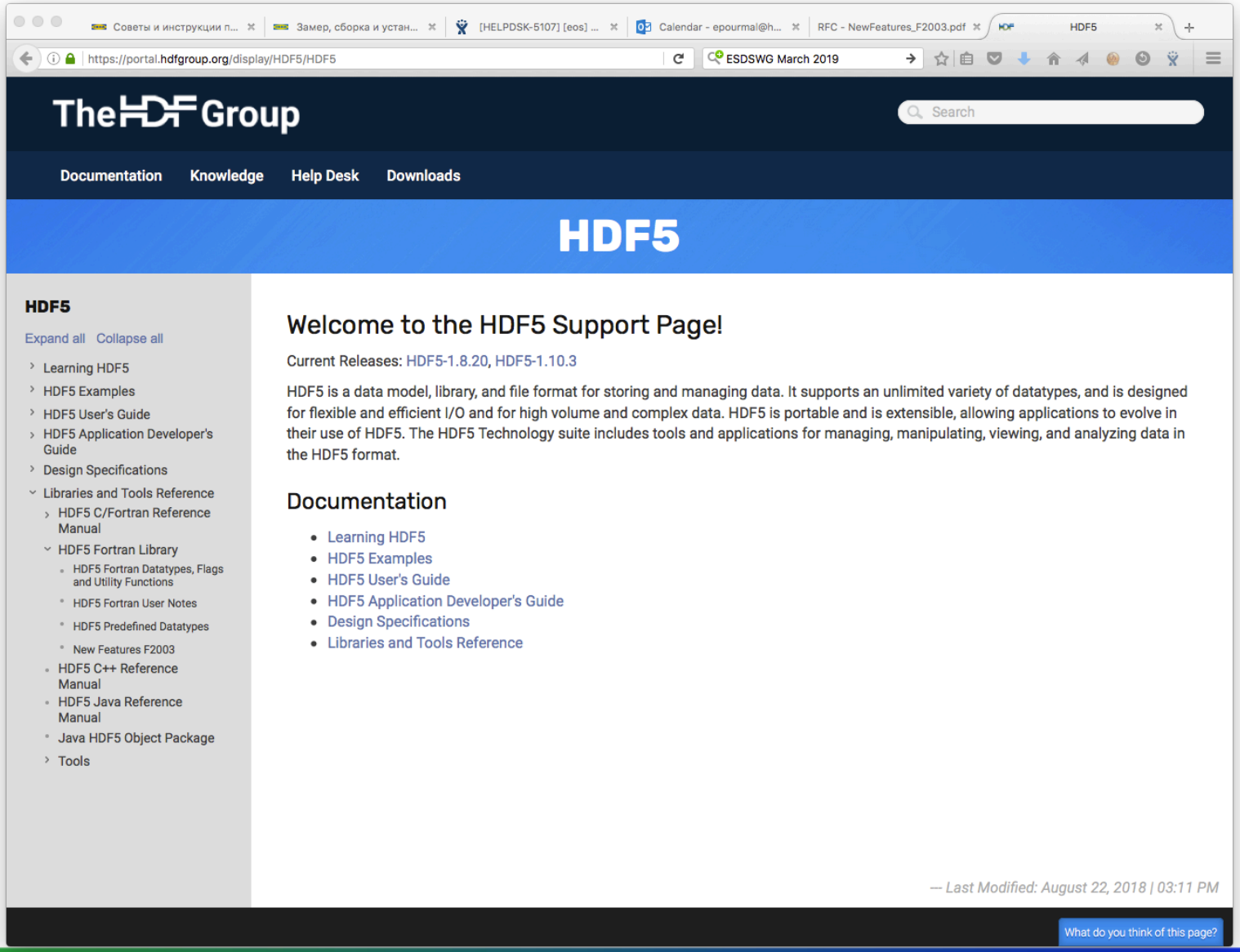
`share` directory

Source code

`fortran/examples` directory

Documentation

https://portal.hdfgroup.org/display/HDF5/HDF5



HDF5 Fortran APIs

- Fortran APIs are organized in modules parallel to the HDF5 Interfaces.
  - USE HDF5 (HDF5 module contains all necessary modules to run HDF5 Fortran application)
- Fortran APIs come in the form of Fortran subroutines:
  - Each Fortran subroutine name is derived from the corresponding C function name by adding "_f" to the name
  - A description of each implemented Fortran subroutine and its parameters can be found the HDF5 Reference Manual.

HDF5 Fortran APIs (cont'd)

- The number and order of the Fortran subroutine parameters may differ from the number and order of the C function parameters.
  - Two additional parameters hold the return value and an error code.
  - Subroutine parameters are listed in the following order:
    - Required input parameters
    - Output parameters, including return value and error code
    - Optional input parameters

Example

C

```
hid_t H5Dcreate(hid_it loc_id, char
*name, hid_t type_id, hid_t space_id,
hid_t creation_prp);
```

Fortran

```
SUBROUTINE h5dcreate_f(loc_id, name,
type_id, space_id, dset_id, hdferr,
creation_prp)
```

Optional parameter, may be omitted if default value is used

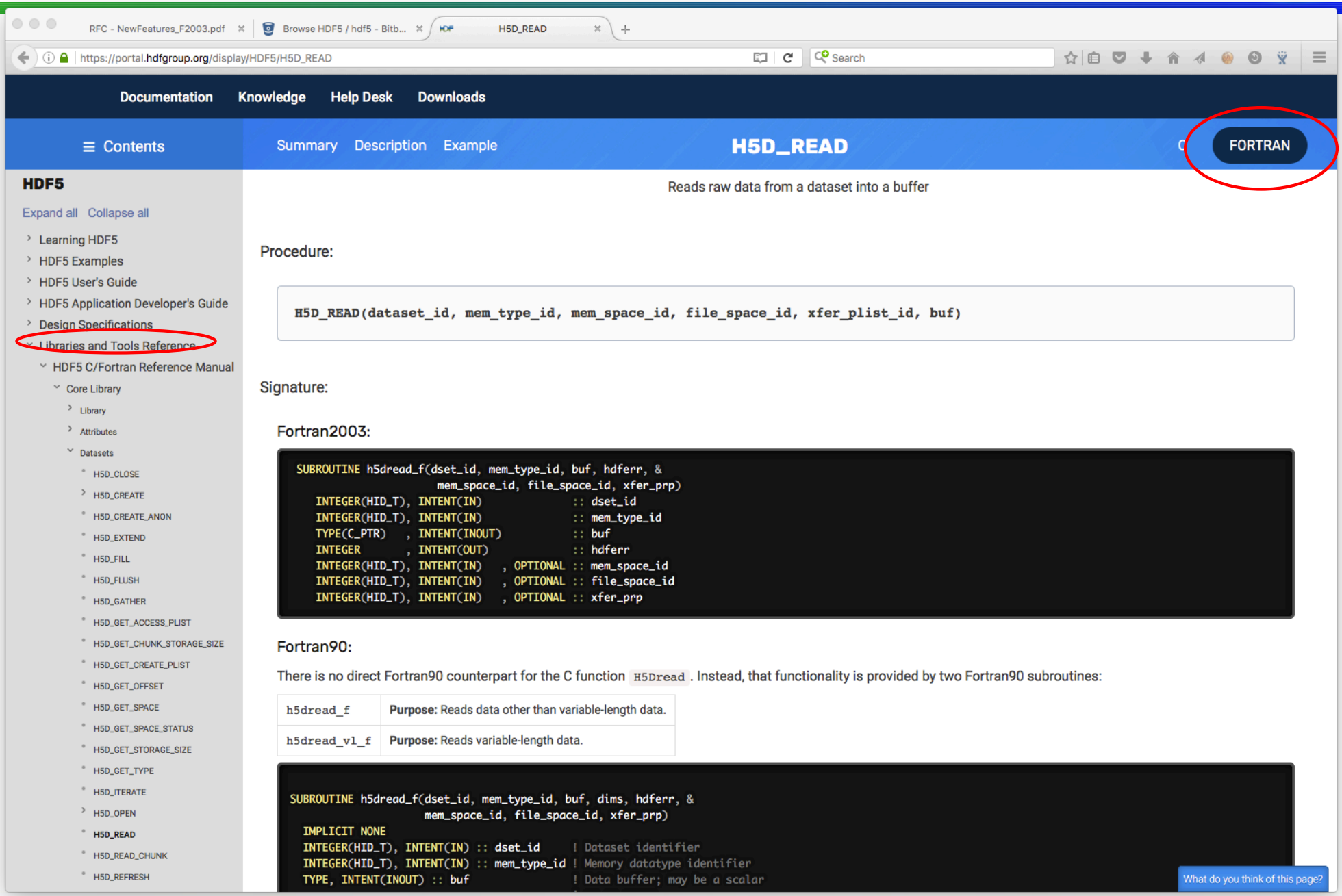
HDF5 F90 and F2003 APIs

- Fortran APIs were introduced in early 2000
  - Based on F90 standard
  - Support for INTEGER, REAL, CHARACTER and DOUBLE PRECISION intrinsic types only
    - No support for INTEGER(KIND=…) and REAL(KIND=...)
    - No support for derived types and enumerated types
  - No support for many HDF5 features, for example,
    - Variable-length datatypes
    - File traversal routines

HDF5 F90 and F2003 APIs (cont'd)

- HDF5 1.10.* versions have F2003 features enabled by default
- Use F2003 APIs to take advantage of HDF5 functionality and to reduce programming effort
- Fortran documentation has both F90 and F2003 signatures
  - Note: Some subroutines do not have F2003 counterparts by design

HDF5 Fortran Documentation



HDF5 F2003 Programming Model

HDF5 Fortran Programming Model

- Each Fortran application must call the h5open_f subroutine to initialize the Fortran interface before calling any HDF5 Fortran subroutine.
- It is a good practice to call the h5close_f subroutine after all calls to the HDF5 Fortran library to close the Fortran interface.
- Fortran indices are 1-based

HDF5 F2003 Programming Model

- To use HDF5 F2003 interfaces follow this programming model in your application:
  - Include the ISO_C_BINDING module
  - Use the following declarations for variable and functions:
    a. Use TARGET attribute in declarations of a variable or an array that contains data to be written or read by the HDF5 Fortran APIs
    b. Use the C_PTR derived data type to declare a pointer to a variable or array in item a.
    c. Use the BIND(C) attribute in derived type declaration

HDF5 F2003 Programming model (cont'd)

- To use HDF5 F2003 interfaces follow this programming model in your application:
    d. Use the BIND(C) attribute in a Fortran callback declaration
    e. C_FUNPTR derived type to declare a pointer to the Fortran function in item d.
- Associate a pointer with a varaible or an array using C_LOC intrinsic datatype, and then pass it to an HDF5 Fortran call
- Associate a pointer with a callback function using the C_FUNCTION intrinsic data type, and then pass it to an HDF5 Fortran call.

Example: Passing a buffer

```
PROGRAM main
    USE ISO_C_BINDING
    USE HDF5
    ...
    TYPE, BIND(C) ::  sensor_t
        ...
    END TYPE sensor_t
    TYPE(sensor_t), DIMENSION(1:100), TARGET :: wdata ! Write buffer
    TYPE(C_PTR) :: ptr
    ...
    ptr = C_LOC(wdata(1))
    CALL h5dwrite_f(dset, memtype, ptr, hdferr)
    ...
END PROGRAM main
```

Fortran 2003: Passing a buffer

In Demo-1 directory:

- Modify `h5_rdwt.f90` to use Fortran 2003 features to simplify h5dwrite(read)_f calls

Example: Passing a call back function

```
PROGRAM main
    USE ISO_C_BINDING
    USE HDF5
! Type iter_info and call op_func function are declared in liter_cb_mod
    USE liter_cb_mod
    ...
    TYPE(C_PTR) :: ptr
    TYPE(C_FUNPTR) :: funptr
    TYPE(iter_info), TARGET ::  info
    ...
    ptr = C_LOC(info)
    funptr = C_FUNLOC(op_func)
    CALL h5literate_f(file, ..., funptr, ptr, ...)
    ...
END PROGRAM main
```

Fortran Language Types vs. HDF5 Datatypes

HDF5 Library Intrinsic Types

- See "HDF5 Fortran Datatypes, Flags and Utility Functions" document.
- For portability HDF5 C library and Fortran wrappers libraries define intrinsic types for parameters declarations; examples:

C type	Fortran type
hid_t	INTEGER(HID_T)
hsize_t	INTEGER(HSIZE_T)
size_t	INTEGER(SIZE_T)

Fortran types vs. HDF5 datatypes

- HDF5 Fortran library provides predefined HDF5 datatypes in form of handles (cmp. with hard coded integers in HDF4) that correspond to the Fortran intrinsic types

Fortran type	HDF5 Fortran type
INTEGER	H5T_NATIVE_INTEGER
REAL	H5T_NATIVE_REAL
CHARACTER	H5T_NATIVE_CHARACTER

- *There are no HDF5 predefined types for kinds of INTEGERS and REALS*
  - Use `h5kind_to_type` function to get HDF5 datatype

Example of using h5kind_to_type

```
INTEGER(SELECTED_INT_KIND (5)), DIMENSION(100), TARGET ::
ivar
….
mem_type = h5kind_to_type(KIND(ivar(1), H5_INTEGER_KIND)
ptr = C_LOC(ivar(1))
CALL h5dwrite_f (dset_t, mem_type, ptr, error)
```

- See h5ex_d_rdwr_kind_F03.f90 in EX-1 directory
- Modify examples `h5_crtdat.f90` and `h5_rdwt.f90` in Demo-1 to use `INTEGER(KIND=8)`

Fortran types vs. HDF5 datatypes

- More on working with Fortran types as we go
  - Derived types (HDF5 compound types)
  - Enum type (HDF5 enum type)
  - Strings
  - Variable-length types

Thank You!

Questions/comments?