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detecting the future

A generic frame-reading API for a runtime-loadable library

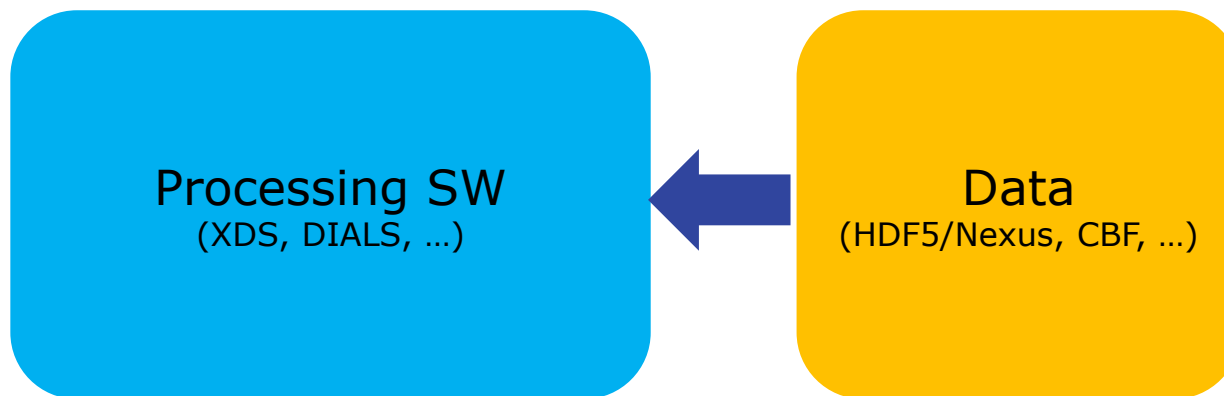
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High Data Rate MX, 26 May 2016***

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Current Situation

- *Efficient processing of data sets requires fast parallel (threaded) reading of a dataset.*
- *Developers of processing software have little resources to keep up with the changes, and little incentive to implement yet another format. Especially the more complex it is.*
- *Users are 😊 about workarounds.*
- *Any new format or change will require adaptations in each software packages consuming this kind of data.*

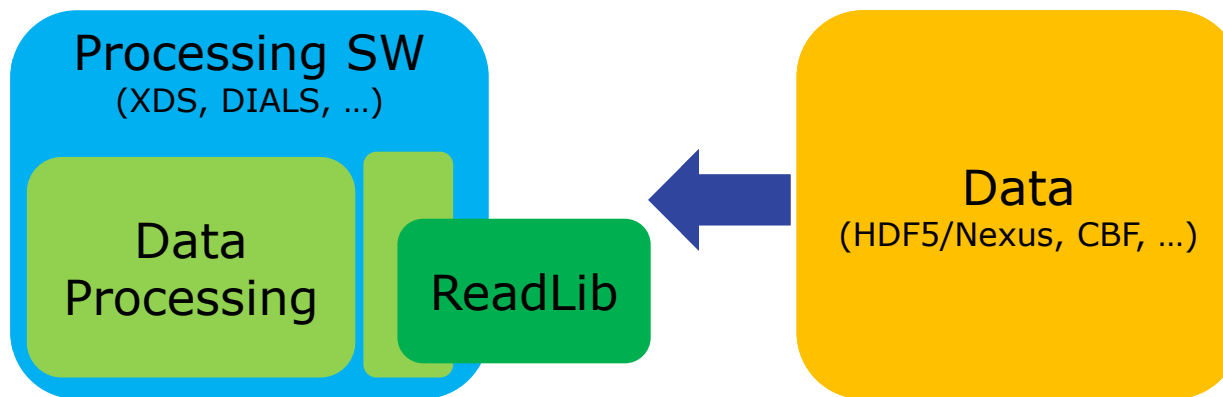


Frame reading in XDS

- *The steps performed by XDS during processing can be cut down to four operations.*
 - *Open a resource providing the frames of a dataset*
 - *Gather information about the contained data*
 - *Get a frame for analysis*
 - *Close the resource*
- *This generalization is not limited to XDS but could also be applied to other programs.*
- *An interoperable (C, Fortran) API with a defined set of functions allows the separation of code for reading and processing.*

Another approach

- A separation between code for reading data and processing data would make everyone's job easier.
- The code for reading data can be physically separated from the code processing data by a plugin mechanism.
- This allows every user to feed the processing software with his data in an optimal way.
- Ideally the community agree on a common set of plugins to ensure reliable usage.



XDS Plugin Mechanism

- XDS loads the library dynamically at runtime using `dlopen/dlsym/dlclose`.*
- The user sets `LD_LIBRARY_PATH` to it. XDS opens the library specified with a “`DETECTOR=libdectrish5toxds`” line in `XDS.INP`, and uses the API-defined routine names.*
- This works for (C, C++ and) Fortran, using Fortran 2003 C interop: see example at <http://cims.nyu.edu/~donev/Fortran/DLL/DLL.Forum.txt>*
- A first version has been integrated into XDS.*

- It is easy to implement a library to read any data.*
- There is a clear separation in code/license ownership.*

This may offer possibilities not hitherto available

- *The library itself can be “signed” (see info array of generic_open_file) by the manufacturer (programmer), and the consumer (data processing program) can check it. The reverse is also true. This may be used to ensure reliable usage.*
- *A way to prevent the faking of data:*
 - *Frames can have their MD5SUM (cryptographically) “signed” by the library (see info array of generic_get_data)*
 - *The consumer program (e.g. XDS) can check the MD5SUM’s integrity*
 - *(Of course this only makes sense if {INTEGRATE,XDS_ASCII}.HKL are also signed, so requires more work to be fully implemented. But it’s a start.)*

Reading HDF5

- *Some notes about HDF5/NeXus*
 - *HDF5/NeXus has been questioned as being a data format suitable for the processing of MX data due to speed reasons*
 - *The hdf5lib has (or at least had) its deficiencies regarding fast parallel reading of data in a threaded environment*
 - *The hdf5lib is the reference implementation of the HDF5 standard. Thus it has to cover the full functionality and backward compatibility.*
- *HDF5/NeXus is for DECTRIS the data format of choice for archiving the data of an experiment and we will make our products compliant with the standard.*

DECTRIS HDF5 Plug-In

- *Two Goals*
 - *Using the plug-in mechanism to speed up processing of HDF5 data with XDS*
 - *Show HDF5 is not bound to the library provided by the HDF5 group as the format is documented*
- *HDF5 plugin*
 - *Does not use any code of the HDF5 group*
 - *Only reads a limited subset of HDF5 data*
 - *DISCLAIMER:*
Proof of principle, far from being production ready code
 - *<https://github.com/dectris/dectris-xds-plugin>*

DECTRIS HDF5 Plug-In

images	CBFs		HDF5	HDF5
DETECTOR=	PILATUS		EIGER	libdectrish5toxds
8 JOBS	152	= total	190	160
8 PROCESSORS	46	= INIT.LP	64	52
	79	= INTEGRATE.LP	99	83
12 JOBS	141		179	152
8 PROCESSORS	47		65	51
	69		88	75
8 JOBS	142		178	157
12 PROCESSORS	46		64	52
	73		89	80
12 JOBS	140		177	151
12 PROCESSORS	46		63	51
	71		89	75
16 JOBS	140		188	153
8 PROCESSORS	46		64	53
	69		96	76

Datensatz: lysoHG4_t0p01_0p1d_0p1s_d150_360deg_master.h5 (Iz4), PSI, 3 Feb 2015
 Dell PowerEdge 930, elapsed wall-clock times for individual steps, all data on RAM disk

Summary

- *One can implement arbitrary data structures (if one has to) AND fast procedures to read them.*
- *This takes away the implementation and maintenance burden from software developers - they can concentrate on improving the precision and accuracy of the data*
- *Logical separation between data and program; enhances modularity; adapts easily to e.g. HDF5-SWMMR*
- *No external program like H5ToXds - no intermediate files needed - no conversion penalties (speed)*
- *Open: API source code is at https://github.com/dectris/dummy_xds_hook*
- *Open: HDF5 plugin proof of principle is at <https://github.com/dectris/dectris-xds-plugin>*

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***Thank you for
your attention!***

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Plug-In API

```
subroutine generic_open(library, template_name, info_array, error_flag)
! Requirements:
! 'LIBRARY'          input  (including path, otherwise using LD_LIBRARY_PATH)
! 'TEMPLATE_NAME'   input  (the resource in image data masterfile)
! 'INFO' (integer array) input  Array of (1024) integers:
!                   INFO(1)    = Consumer ID (1:XDS)
!                   INFO(2)    = Version Number of the Consumer software
!                   INFO(3:8)  = Unused
!                   INFO(9:40) = 1024bit signature of the consumer software
!                   INFO(>41)  = Unused
! 'INFO' (integer array) output Array of (1024) integers:
!                   INFO(1)    = Vendor ID (1:Dectris)
!                   INFO(2)    = Major Version number of the library
!                   INFO(3)    = Minor Version number of the library
!                   INFO(4)    = Parch Version number of the library
!                   INFO(5)    = Linux timestamp of library creation
!                   INFO(6:8)  = Unused
!                   INFO(9:40) = 1024bit signature of the library
!                   INFO(>41)  = Unused
! 'ERROR_FLAG'      output Return values
!                   0 Success
!                   -1 Handle already exists
!                   -2 Cannot open Library
!                   -3 Function not found in library
!                   -4 Master file cannot be opened (coming from C function)
!                   -10 Consumer identity not supported (coming from C function)
!                   -11 Consumer identity could not be verified (coming from C function)
!                   -12 Consumer software version not supported (coming from C function)
```

Plug-In API

```
subroutine generic_get_header(nx, ny, nbyte, qx, qy, number_of_frames, info_array, error_flag)
! Requirements:
! 'NX' (integer)          output  Number of pixels along X
! 'NY' (integer)          output  Number of pixels along Y
! 'NBYTE' (integer)       output  Number of bytes in the image... X*Y*DEPTH
! 'QX' (4*REAL)           output  Pixel size
! 'QY' (4*REAL)           output  Pixel size
! 'NUMBER_OF_FRAMES' (integer) output  Number of frames for the full dataset. So far unused
! 'INFO' (integer array)  input   Array of (1024) integers:
!                          INFO(>1)   = Unused
! 'INFO' (integer array)  output  Array of (1024) integers:
!                          INFO(1)     = Vendor ID (1:Dectris)
!                          INFO(2)     = Major Version number of the library
!                          INFO(3)     = Minor Version number of the library
!                          INFO(4)     = Patch Version number of the library
!                          INFO(5)     = Linux timestamp of library creation
!                          INFO(6:64)  = Reserved
!                          INFO(65:1024) = Dataset parameters
! 'ERROR_FLAG'           output  Return values
!                          0           Success
!                          -1          Cannot open library
!                          -2          Cannot read header (will come from C function)
!                          -4          Cannot read dataset informations
!                                     (will come from plug-in function)
!                          -10         Error in the determination of the Dataset parameters
!                                     (will come from plug-in function)
!
```

Plug-In API

```
subroutine generic_get_data(frame_number, nx, ny, data_array, info_array, error_flag)
! Requirements:
! 'FRAME_NUMBER' (integer)      input  Number of frames for the full dataset. So far unused
! 'NX' (integer)                input  Number of pixels along X
! 'NY' (integer)                input  Number of pixels along Y
! 'DATA_ARRAY' (integer array)  output  1D array containing pixel data with length = NX*NY
! 'INFO' (integer array)        output  Array of (1024) integers:
!                               INFO(1)      = Vendor ID (1:Dectris)
!                               INFO(2)      = Major Version number of the library
!                               INFO(3)      = Minor Version number of the library
!                               INFO(4)      = Patch Version number of the library
!                               INFO(5)      = Linux timestamp of library creation
!                               INFO(6:8)    = Unused
!                               INFO(9:40)   = 1024bit verification key
!                               INFO(41:44)  = Image MD5 Checksum
!                               INFO()       = Unused
! 'ERROR_FLAG' (integer)        output  Provides error state condition
!                               0 Success
!                               -1 Cannot open library
!                               -2 Cannot open frame (will come from C function)
!                               -3 Datatype not supported (will come from C function)
!                               -4 Cannot read dataset informations (will come from C function)
!                               -10 MD5 Checksum Error
!                               -11 Verification key error
!
```