Parallel HDF5 and compression filters with synchrotron scattering data

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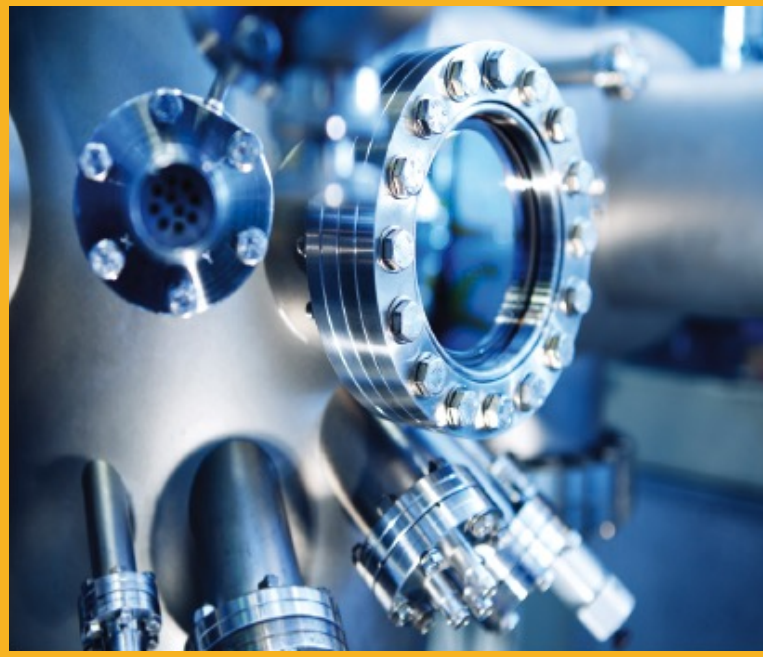
Ingredients

- parallel HDF5 with MPI
- image like synchrotron data
- compression

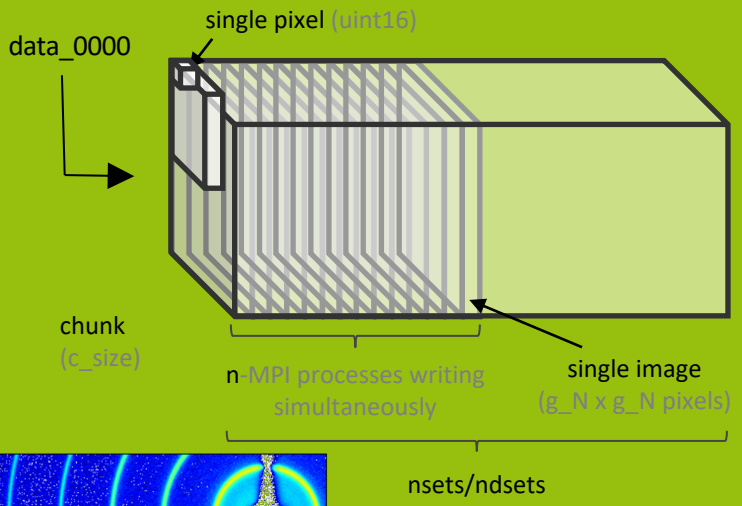


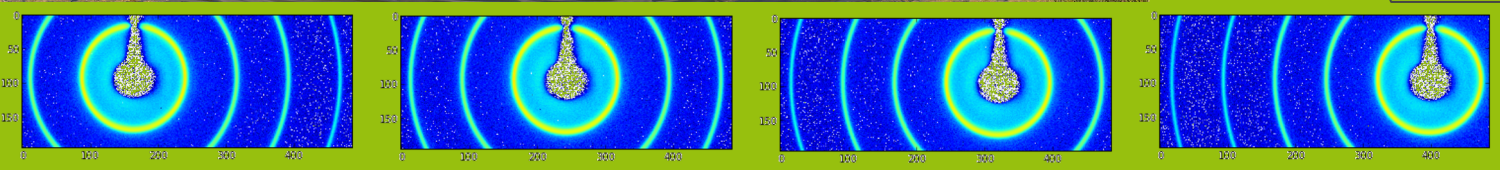
Parallel HDF5 with MPI

- message passing interface (MPI) is a **standard for parallel computing** architecture; invented in 1991-1992; popular at high-performance-computing (HPC) clusters
- Sophie Servan (DESY) et al., **Technical-Workshop-Survey (2020)**: 9/10 facilities have SLURM HPC cluster
  https://github.com/ExPaNDS-eu/ExPaNDS/blob/master/WP4/20201009-Technical-Workshop-Survey.pdf
- "reference" HDF5 library implementation
  - a complex sw with numerous technical limitations one should be aware of
  - MPI enables distributed multi-task application can effectively read/write data to a single HDF5 file and even to a single dataset
  - well defined parallel HDF5 library and compatible software (h5py/mpi4py) are available off-the-shelf in HPC sw distributions (e.g. EasyBuild)
  - parallel HDF5 is a "traditional" feature, i.e. 1.8
  - **sw**: savu (Diamond), PtyPy - both are mpi4py & h5py
- alternatives with serial HDF5
  - virtual datasets distributed over multiple files
  - direct chunk write/read
  - disadvantage: 1.10 required, some sw cannot read such data

Image like synchrotron data

- general synchrotron data have complex structure&format
- “detector” data (99% volume of all data): usually 2D or 3D datasets
- here focus on performance
  - example JungFRAU detector (PSI)
    - 4M pixels (2 bytes depth) x 2 kHz
    - **16 GB/s** uncompressed, **bslz4 compression factor ~ 4x**, finally 4 GB/s compressed





pHDF5, image like data, no compression

tools

- tools: h5perf_parallel, ior (`-a HDF5`), hdf5_pwrite3dc, h5py-snippets/gist
- hdf5_pwrite3dc is deeply inspired by code from *Timoty Brown* on Stackoverflow

```python
from mpi4py import MPI
import h5py
import numpy as np
import sys

def _create_dataset_nofill(group, name, shape, dtype, chunks=None):
    spaceid = h5py.h5s.create_simple(shape)
    plist = h5py.h5p.create(h5py.h5p.DATASET_CREATE)
    plist.set_fill_time(h5py.h5d.FILL_TIME_NEVER)
    if chunks not in [None,[]] and isinstance(chunks, tuple):
        plist.set_chunk(chunks)
    typeid = h5py.h5t.py_create(dtype)
    datasetid = h5py.h5d.create(group.file.id, group.name+'/'+name, typeid, spaceid, plist)
    dset = h5py.Dataset(datasetid)
    return dset

n_frames = 6000
ch_n = g_n = 4096
comm = MPI.COMM_WORLD # common communicator
n_tasks = comm.size # number of tasks
rank = comm.rank # process ID

# prepare local data
data = np.ones((g_n,g_n),dtype=np.int32)

# set collective transport property
dxpl = h5py.h5p.create(h5py.h5p.DATASET_XFER)
dxpl.set_dxpl_mpio(h5py.h5fd.MPIO_COLLECTIVE)

f = h5py.File(sys.argv[1], 'w', driver='mpio', comm=MPI.COMM_WORLD)

dset = _create_dataset_nofill(f['/'],'test', (n_frames, g_n, g_n), dtype=np.int32, chunks=(1, ch_n, ch_n))

for i in np.arange(rank,n_frames,n_tasks):
    data += i
    dset[i] = data

f.close()
```

workaround to set FILL_TIME_NEVER in h5py
h5py issue #1282

code

pHDF5, image like data, no compression

typical figures

	compression	write [GB/s]	read [GB/s]	ntasks	comment
ior	no	5.7	4.1	8	1 x FDR
pwrite	no	5.8	4.8	8	1 x FDR
pwrite	no	10.9	8.2	8	2 x FDR
h5py-parallel	no	4.5	-	16	1 x FDR
h5py-serial (dask)	no	-	5.4	16	1 x FDR

- Nice ! It works. Write/read rates limited mainly by bandwidth to storage.

pHDF5, image like data, compression filter

typical figures

	compression	write [GB/s]	read [GB/s]	ntasks (omp)	comment
pwrite	no	5.8	4.8	8	1 x FDR
pread-eiger	bslz4	-	23.8 ✓	20(2)	compression rate: **8.1**
pwrite-bslz4	bslz4	4.9 (?)	-	24(2)	compression rate: 8.1

- Table: “raw” i.e. uncopressed data rates
- 4.9 / 8.1 ~ 0.6 GB/s - storage is likely not a bottleneck
- bslz4 compression is very effective, in particular at least 2x faster
- uncompressed write faster than compressed, read OK
- with multiple files, VDS, in-memory bslz4 compression and direct chunk write better performance can be achived

- parallel HDF5 is great but writing data with compression-filters is not so shiny (?)