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Advances in IO and compilation configuration (HDF5 successful implementation)

(Pencil Code User Meeting, Lausanne/Switzerland, 19th of May 2021)

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Overview:

* Comparison of IO modules

* Features of HDF5

* Conversion tool now available => pc_convert_hdf5.pro

* pc_build => now automatically detects MPI/non-MPI runs and chooses the right compiler

Collective IO and ghost cells

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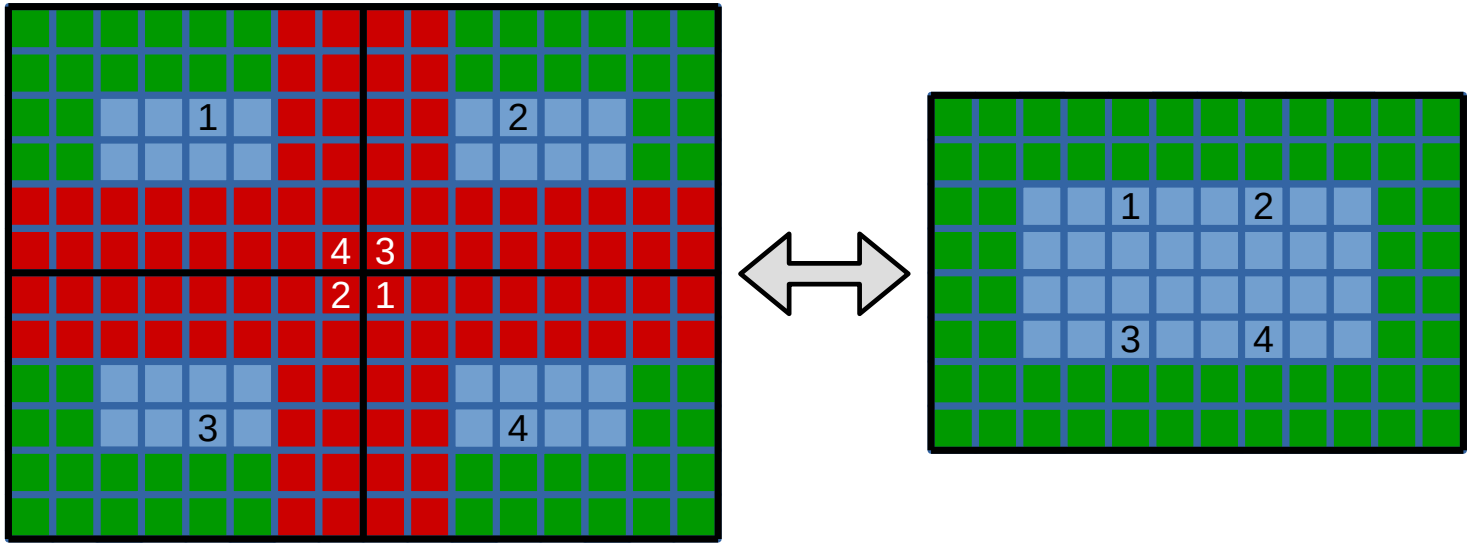

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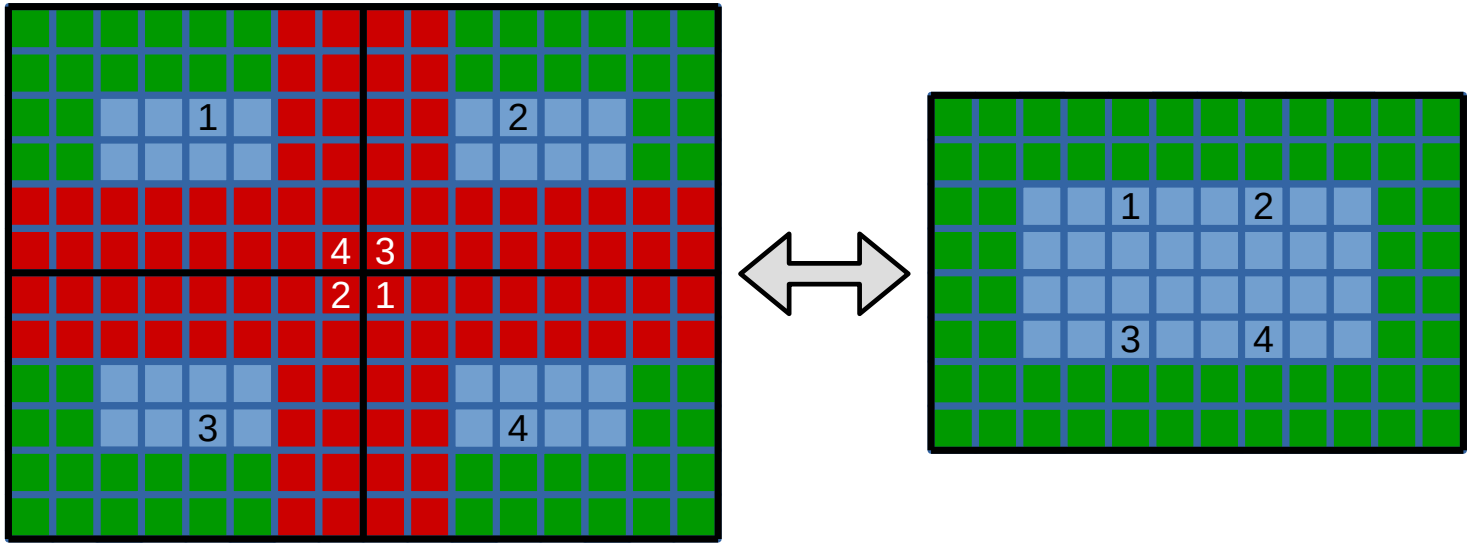
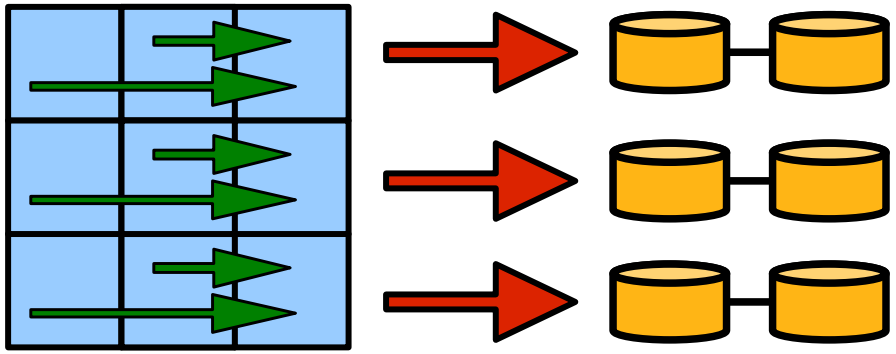


- **io_collect_xy**: collect data on special IO nodes; not all ghost cells removed:



How to install and use HDF5?

- On ubuntu systems, just install the packages:

  “**libhdf5-openmpi-dev**“ (mandatory)

  “**h5tools**” (optional), “**hdfview**” (optional)

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  “**module load ...hdf5...**” (check „**module avail**“ for available packages)

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- Change “src/Makefile.local” (see “samples/corona” for an example):

  IO = io_hdf5

  => „pc_build“ will then automatically find the HDF5 compiler wrapper.

Massive parallel file access

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What is possible regarding IO? **1024*1024*256:**

- “io_dist.f90“ writes distinct files from each processor **2 s**

  (fastest, filesystem heavily loaded, stores all inner ghost cells)

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- “io_collect.f90“ collects everything on one processor **70 s**
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- “io_collect_xy.f90“ collects everything on the xy-leading processor **10 s**
  (still fast also for many processors, stores some inner ghost cells)

- “io_mpi.f90“ collects everything using available processors **8 s**
  (fast, binary format, requires self-written PC reading routines)

- “io_hdf5.f90“ collects everything using all processors **9 s**
  (fast, self-explaining extendible data format, readable everywhere)

What is possible regarding IO? 512*512*512:

Run #		io_ref	io_dist	io_hdf5	io_collect	io_collect_xy	io_mpi2	wall times [h]
	1	0.12600	0.08774	0.27500	0.16100	0.08233	0.36800	
	2	0.06799	0.08130	0.31300	0.22100	0.14100	0.34600	
	3	0.06032	0.07303	0.29600	0.21900	0.09754	0.32100	
	4	0.03970	0.06528	0.24700	0.22200	0.10700	0.33400	
	5	0.04528	0.08753	0.28700	0.18300	0.04515	0.34800	
mean value		0.06786	0.07898	0.28360	0.20120	0.09460	0.34340	[h]
standard deviation		0.03442	0.00973	0.02471	0.02779	0.03504	0.01749	[h]
relative fluctuation		51 %	12 %	9 %	14 %	37 %	5 %	
fastest run		0.0397	0.06528	0.247	0.161	0.04515	0.321	[h]
snapshots			20	20	20	20	20	
time per snapshot			4.6044	37.314	21.834	0.981	50.634	[s]
speed loss			1,00	8,10	4,74	0,21	11,00	
confidence interval		0,01995	0,00564	0,01433	0,01611	0,02031	0,01014	

=> large fluctuations & **io_collext_xy** faster than **io_dist**!?

What is possible regarding IO? 512*512*512:

Run #		io_ref	io_dist	io_hdf5	io_collect	io_collect_xy	io_mpi2	wall times [h]
	1	0.006466	0.01236	0.19500	0.102	0.02359	0.230	
	2	0.005980	0.01193	0.19400	0.102	0.02694	0.226	
	3	0.005525	0.01374	0.19800	0.103	0.02512	0.222	
	4	0.005762	0.01163	0.19500	0.106	0.03220	0.224	
	5	0.005981	0.01229	0.19300	0.106	0.03808	0.223	
	6	0.005197	0.01308	0.18900	0.106	0.02451	0.230	
	7	0.005073	0.01443	0.19100	0.106	0.03448	0.226	
	8	0.005651	0.01263	0.19400	0.105	0.04865	0.224	
	9	0.004900	0.01278	0.19600	0.102	0.02783	0.224	
	10	0.005846	0.01178	0.20200	0.103	0.03184	0.224	
mean value		0.00564	0.01267	0.19470	0.10410	0.03132	0.22530	[h]
standard deviation		0.00048	0.00089	0.00359	0.00185	0.00770	0.00275	[h]
relative fluctuation		8 %	7 %	2 %	2 %	25 %	1 %	
fastest run		0.0049	0.01163	0.189	0.102	0.02359	0.222	[h]
snapshots			20	20	20	20	20	
time per snapshot			1.2114	33.138	17.478	3.3642	39.078	[s]
speed loss			1,00	27,36	14,43	2,78	32,26	
confidence interval		0,00028	0,00051	0,00208	0,00107	0,00446	0,00159	

=> less fluctuations, but obviously **not an optimal setup** (huge differences)...

IO abstraction layer for HDF5

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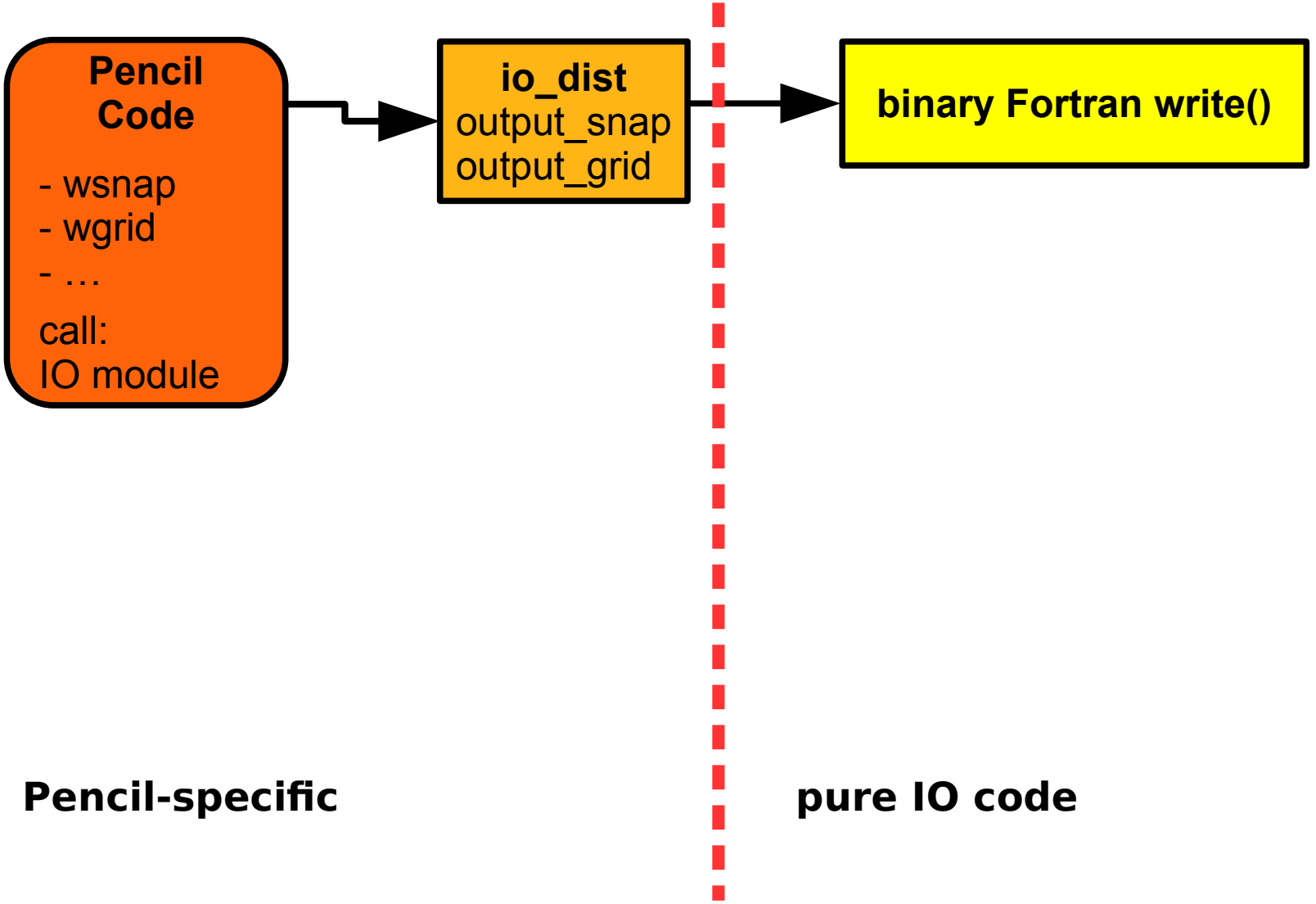
Separation of Pencil-specific code from IO code:



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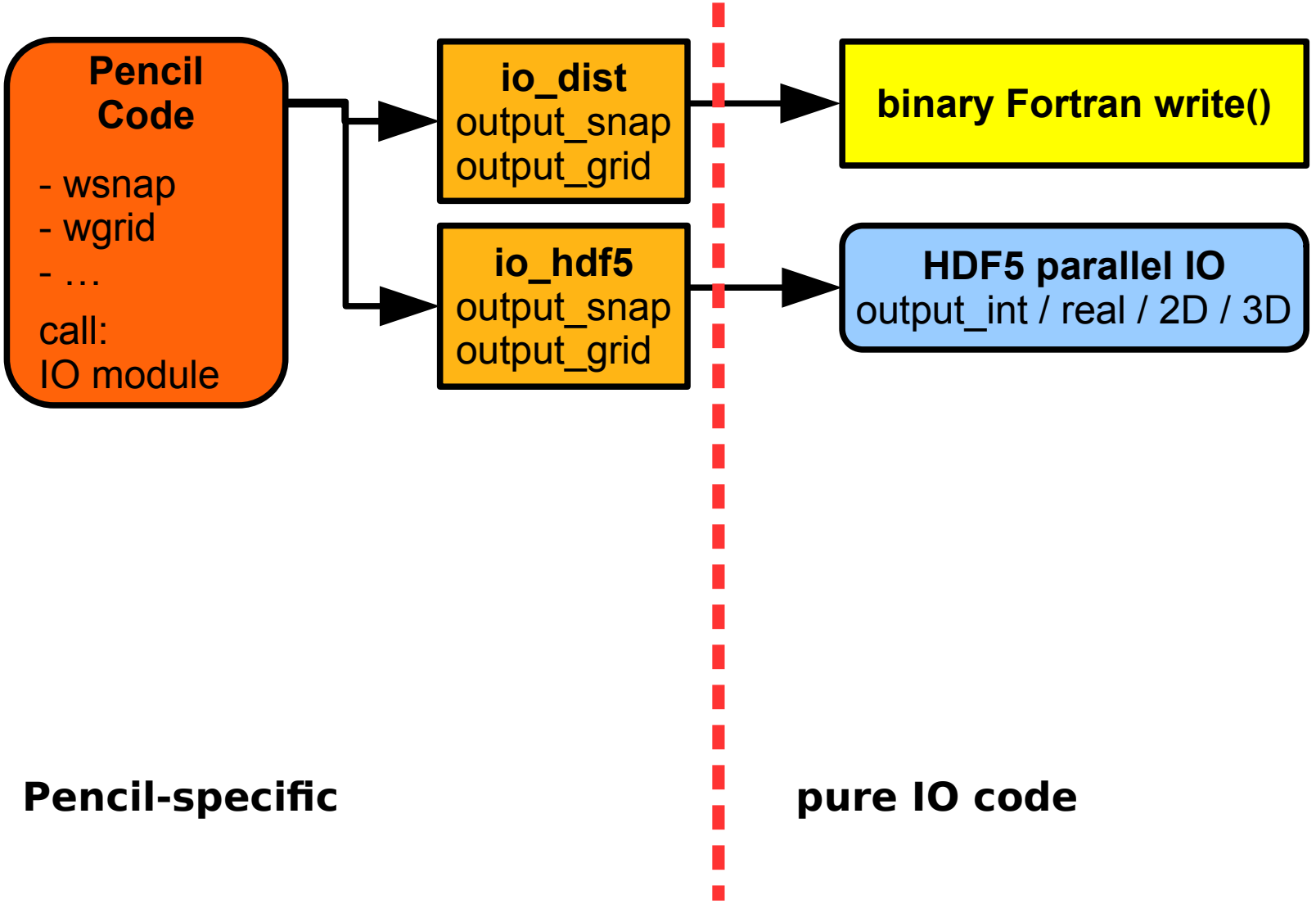

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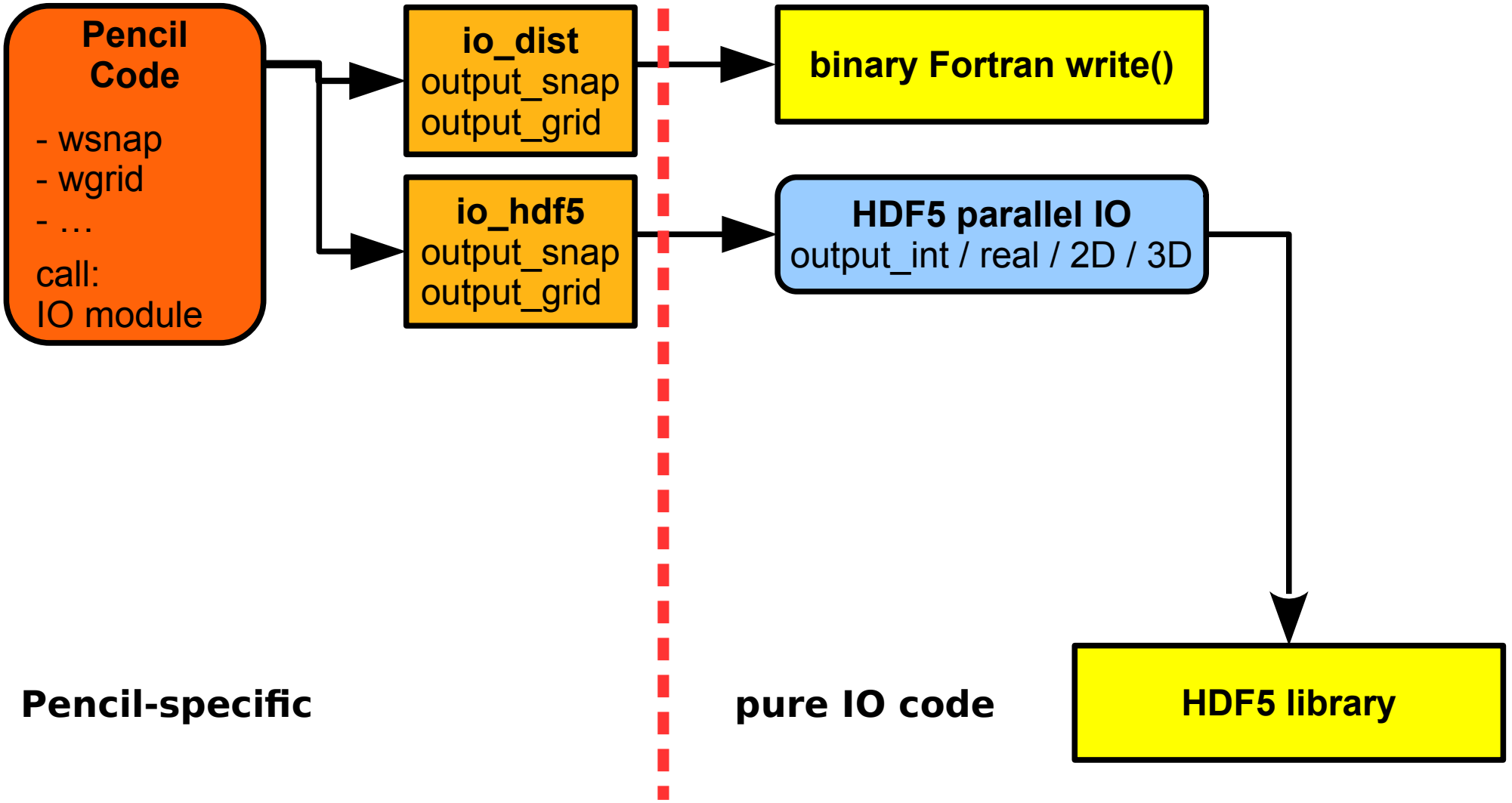

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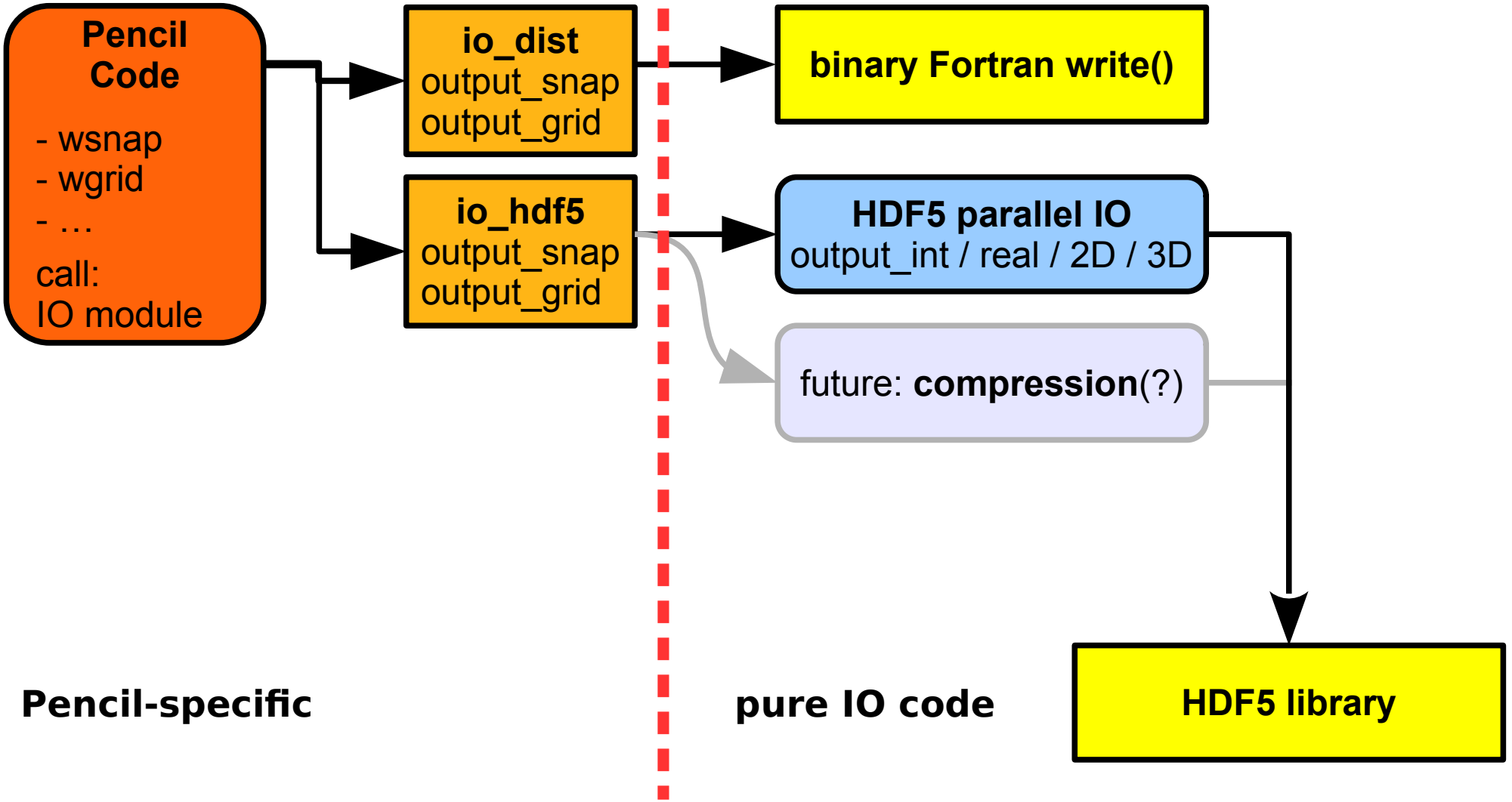

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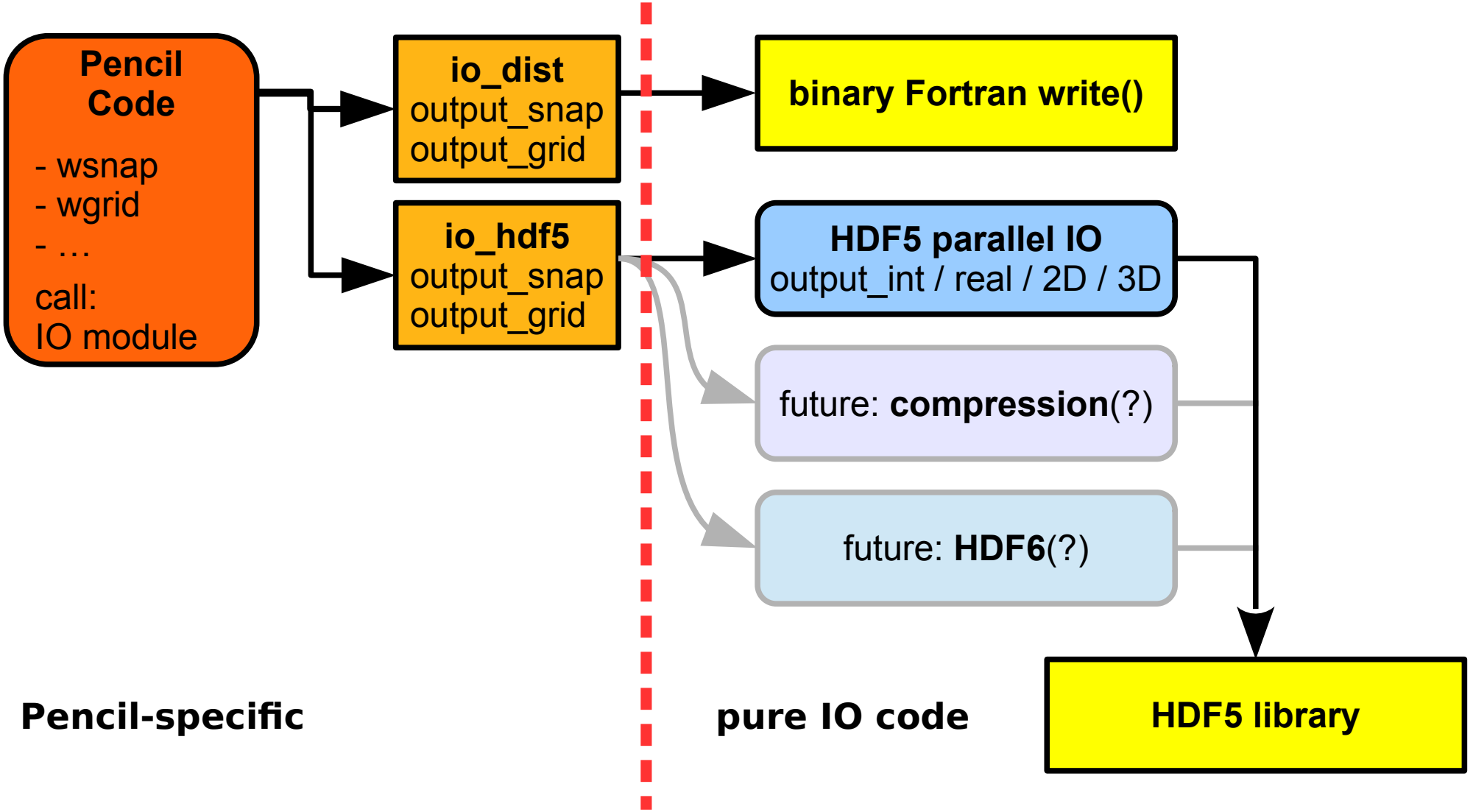

Large-scale data processing

Why using collective snapshot files?

- IDL is slow in reading and combining distributed varfiles

- Using structures in IDL requires much more resources (memory, CPU)

- Inner ghost layers don't need to be stored (can save up to 50%)

How to read HDF5 snapshots in IDL?

- Important IDL routines automatically switch to use HDF5, if available:

  pc_read_var, pc_read_var_raw, pc_read_slice, pc_read_subvol_raw,
  pc_read_grid, pc_read_dim, pc_read_ts, pc_read_video,
  pc_read_pvar, pc_read_qvar, pc_read_pstalk,
  pc_get_quantity, pc_read_xyaver, pc_read_phiavg, ...

- New unified IDL reading routine “pc_read” for HDF5 snapshots:

```
Ax = pc_read ('ax', file='var.h5')     ;; open file 'var.h5' and read Ax
Ay = pc_read ('ay', /trim)             ;; read Ay without ghost cells
Az = pc_read ('az', processor=2)       ;; read data of processor 2
ux = pc_read ('ux', start=[47,11,13], count=[16,8,4]) ;; read subvolume
aa = pc_read ('aa')                    ;; read all three components of vector-field A
xp = pc_read ('part/xp', file='pvar.h5')       ;; get x position of particles
ID = pc_read ('stalker/ID', file='PSTALK0.h5')    ;; stalker particle IDs
```

Read and write HDF5 files IDL

- Low-level routines for basic needs:

idl/read/hdf5/	h5_open_file	open HDF5 file (read, write, or truncate)
	h5_contains()	returns true if a given dataset exists
	h5_content()	returns all dataset names in a group
	h5_get_size()	returns the size of a dataset
	h5_get_type()	returns the IDL type of a dataset
	h5_read()	returns the content of a dataset
	h5_write	write a dataset
	h5_create_group	create a dataset group
	h5_close_file	close HDF5 file

=> If possible, use a high-level function like „pc_read()“ instead!

Improved capabilities on secondary outputs:

- Averages are always consistent after restarts from earlier snapshots.

- Videofiles are always consistent, too.

- No need anymore for „pc_read_all_videofiles“ and similar.

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Outlook:

- Conversion tool using „pc_read_var“ and storing HDF5 with „h5_write“?
  (and similar for “pc_read_pvar / _qvar / _pstalk“)

How to view HDF5 snapshots directly?

- In a terminal:

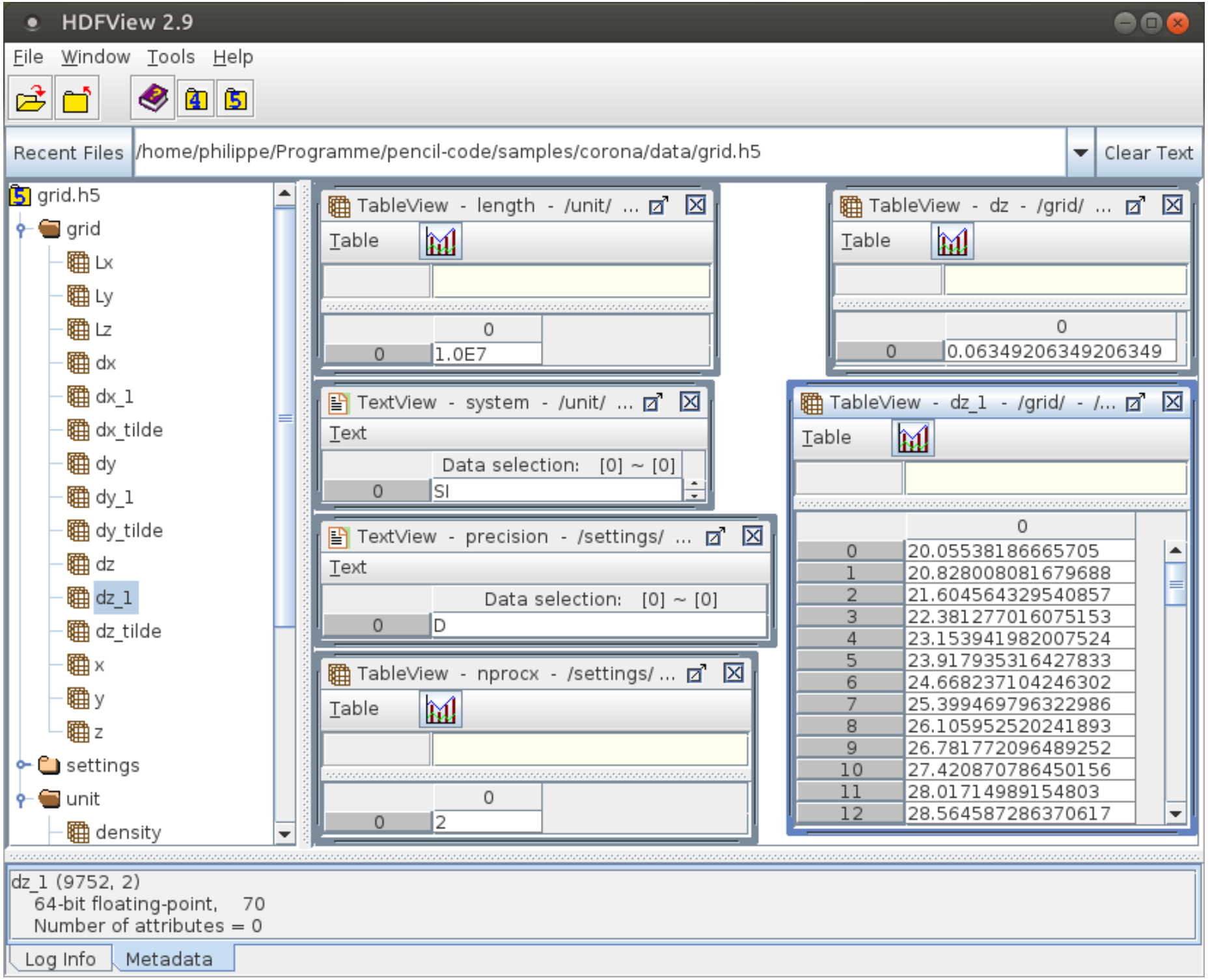
    h5dump -H file.h5

- Graphical tool:

    hdfview file.h5

- Other:

    Matlab, Tecplot, ParaView, etc. directly load and display HDF5 data


HDFView 2.9
File Window Tools Help
Recent Files
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6 24.668237104246302
7 25.399469796322986
8 26.105952520241893
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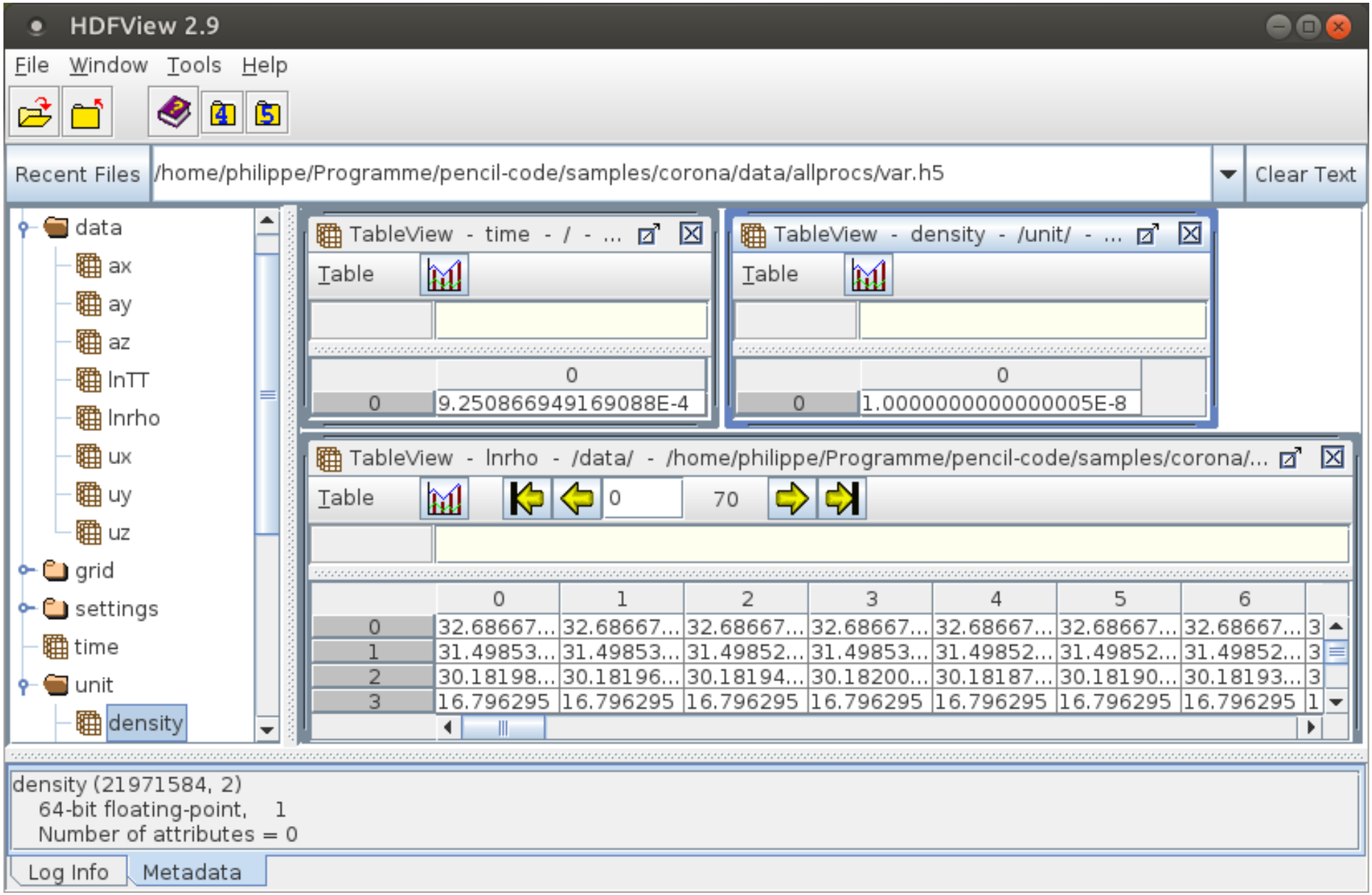
Log Info
Metadata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density (21971584, 2)
64-bit floating-point, 1
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Thank you for supporting the HDF5 transition!