- Log into scinet with your account:
  - `ssh -Y hpcsioXX@login.scinet.utoronto.ca`
  - `ssh -Y gpc01`
  - `qsub -X -I -l nodes=1:ppn=8,walltime=4:00:00`
  - `cd ${SCRATCH}`
  - `cp -r /scinet/course/parIO .`
  - `cd parIO`
  - `source parallellibs`

Parallel I/O

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Agenda

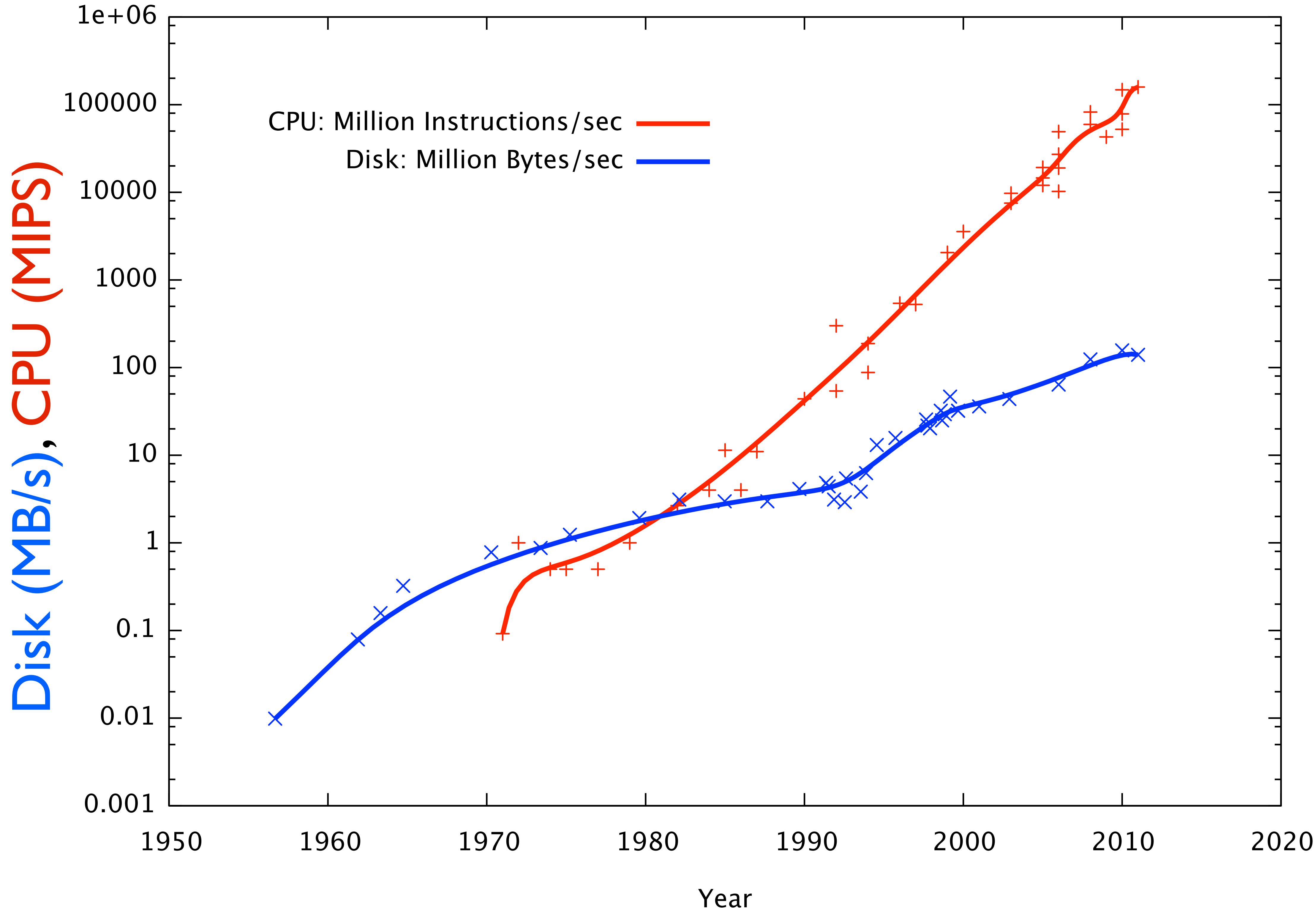
- Intro to I/O
- MPI-IO
- HDF5, NetCDF4
- Parallel HDF5/NetCDF4
- ADIOS (?)

Data is getting bigger

- Increase in computing power makes simulations larger/more frequent
- Increase in sensor technology makes experiments/ observations larger
- Data sizes that used to be measured in MB/GB now measured in TB/PB.
- Easier to generate the data than to store it:

Economist, 27 Feb 2010

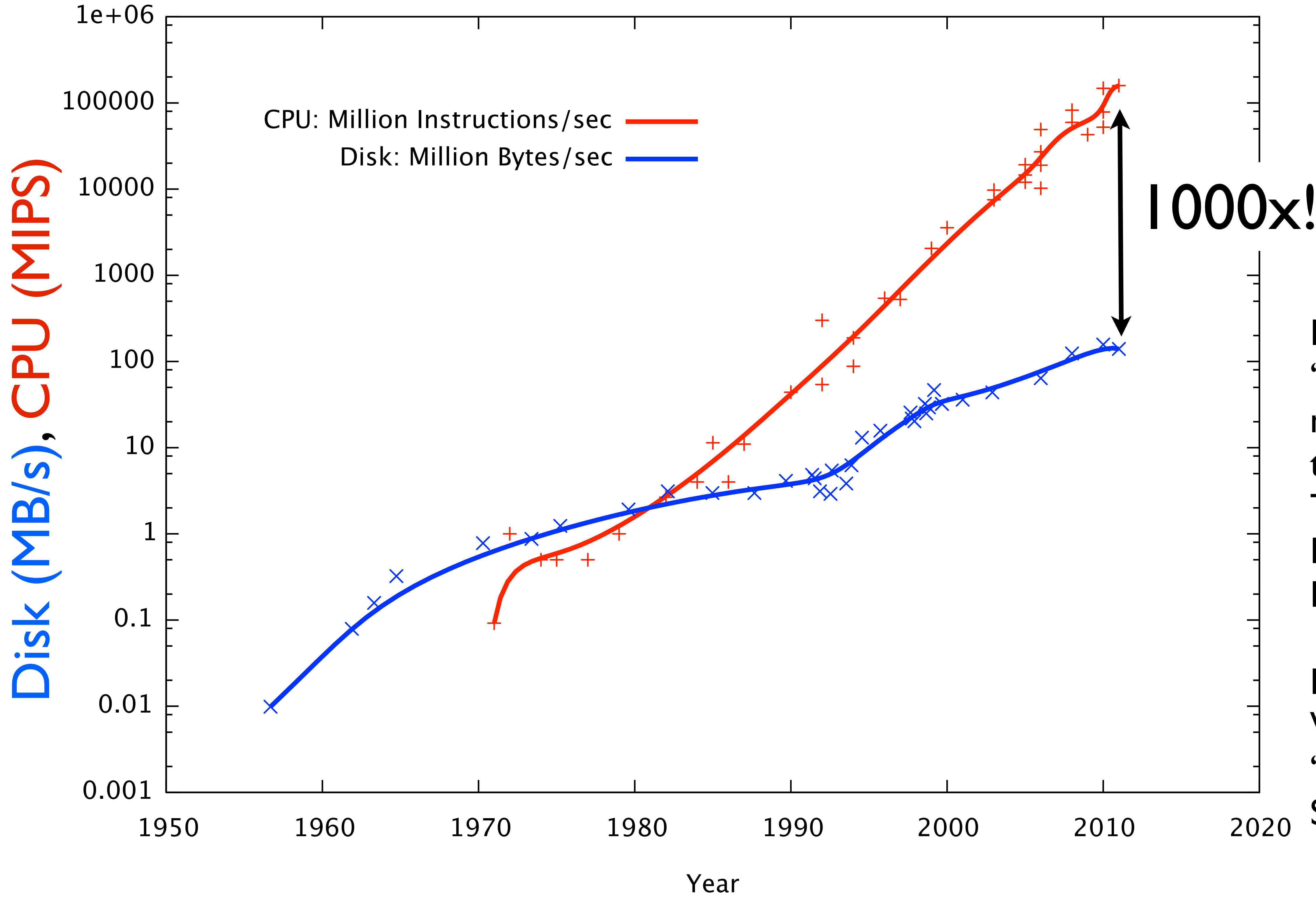
Disks are slower than CPUs (and getting slower)



Disk data from "The future of magnetic storage technology", Thompson & Best, and Tom's Hardware;

MIPS data from Wikipedia, "Instructions per Second".

Disks are slower than CPUs (and getting slower)



Disk data from "The future of magnetic storage technology", Thompson & Best, and Tom's Hardware;

MIPS data from Wikipedia, "Instructions per Second".

Understanding storage performance

- Data rate: MB/s
  - Peak or sustained
  - Write faster than read
  - Network analogy: bandwidth
- IOPS: I/O Operations Per Second
  - open, close, seek, read, write
  - Network analogy: 1/latency

Understanding storage performance

Device	Bandwidth (MB/s)	IOPS
SATA HDD	100	100
SSD	250	10000

HD:

Open, Write, Close 1000x1kB files: 30.01s (eff: 0.033 MB/s)

Open, Write, Close 1x1MB file: 40ms (eff: 25 MB/s)

Understanding storage performance

Device	Bandwidth (MB/s)	IOPS
SATA HDD	100	100
SSD	250	10000

SSD:

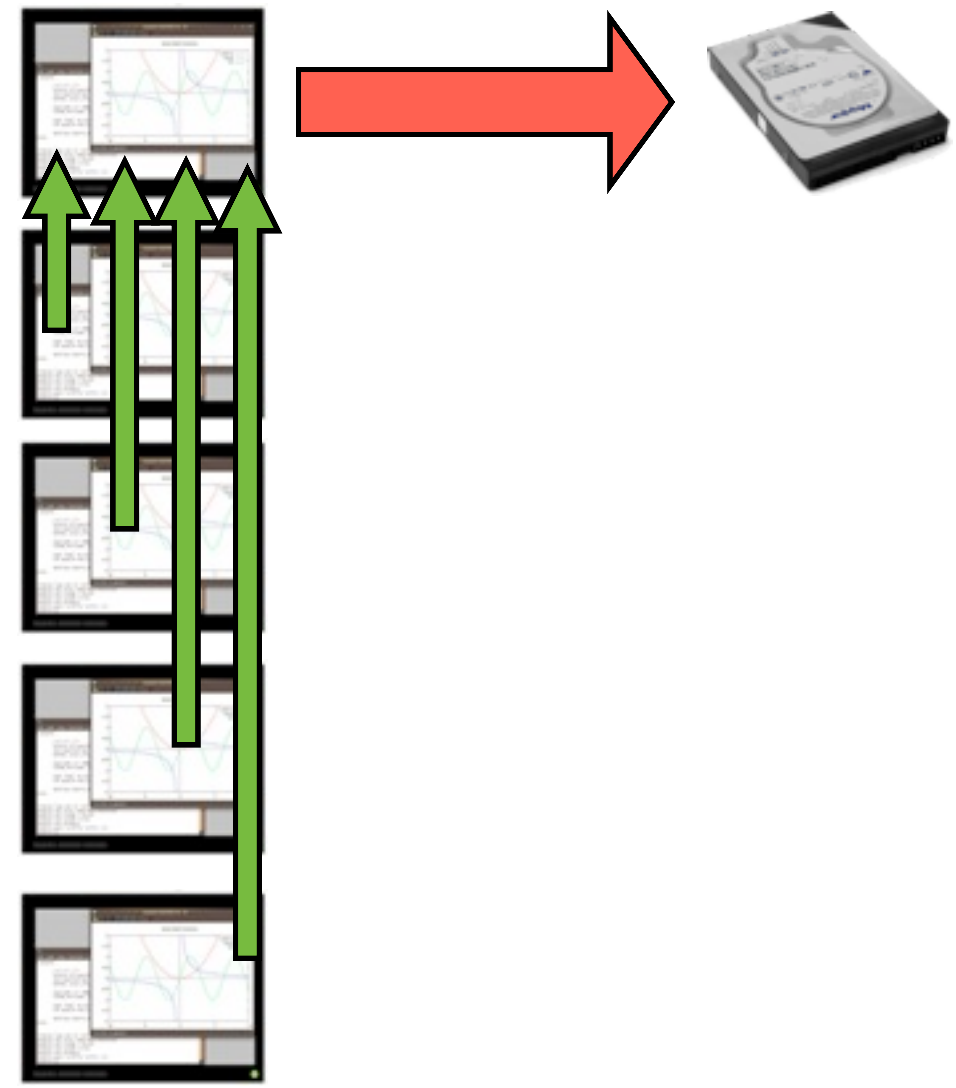
Open, Write, Close 1000x1kB files: 300ms (eff: 3.3 MB/s)

Open, Write, Close 1x1MB file: 4ms (eff: 232 MB/s)

Understanding storage performance

- SSDs are much faster at IOPS:
  - No physical mechanisms that must move to file position
  - Read ~ as fast as write
- But still latency at controller, system calls, etc.
- SSDs will always be much more expensive than disk per unit storage - disk isn't going away.

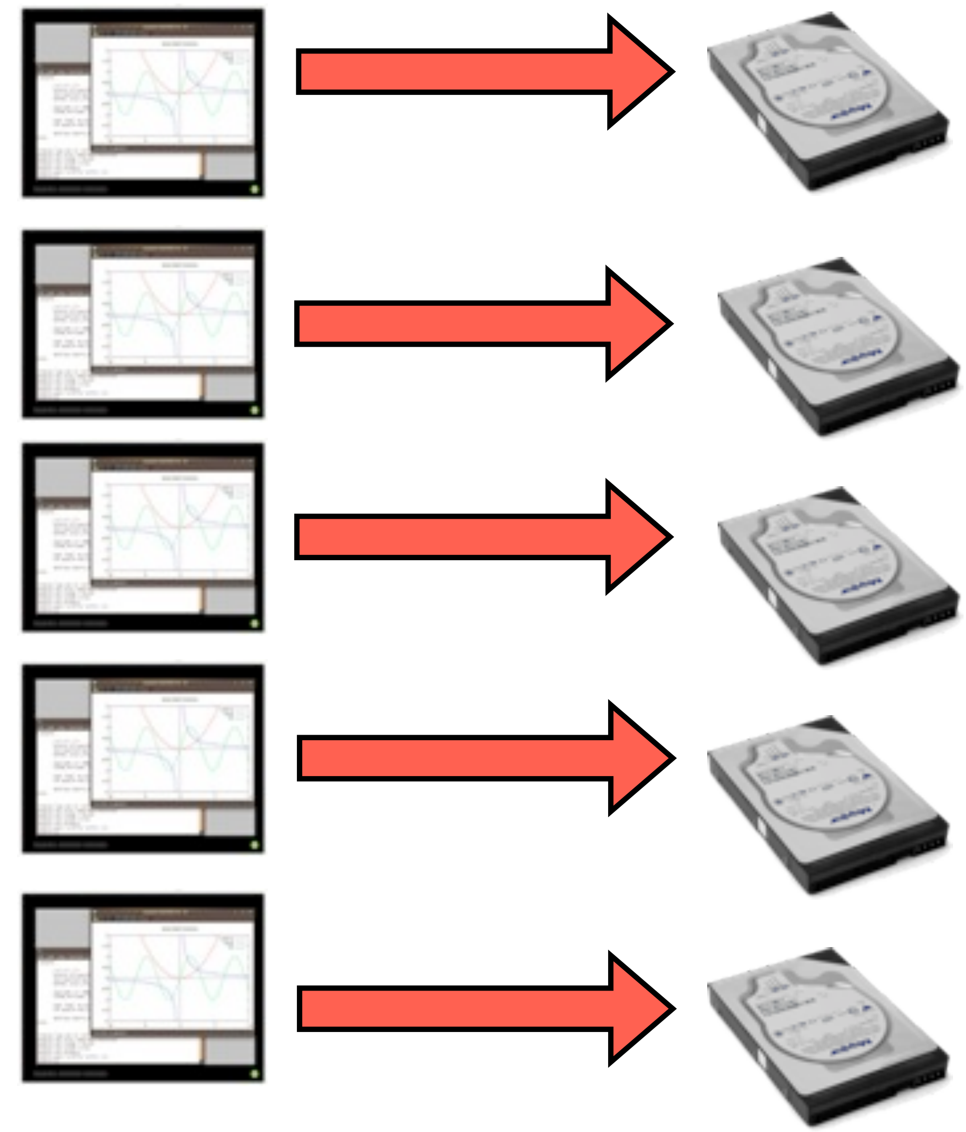
Planning your I/O



- Parallel computation, several options.
- Everyone sends data to process 0
- Process 0 writes.
- Serialize I/O - huge bottleneck.

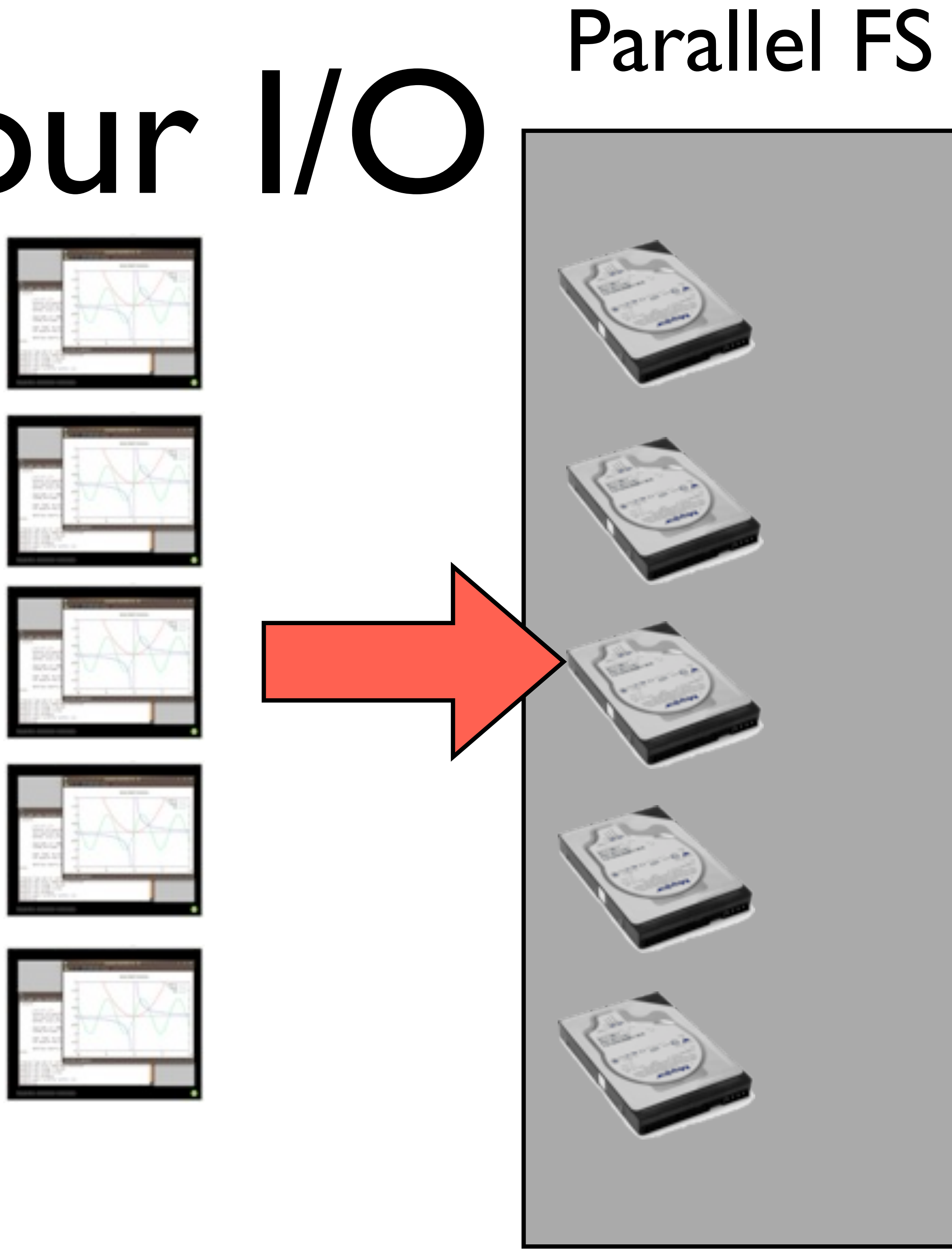
Planning your I/O

- Parallel computation, several options.
- Each process writes a file, possibly to local disk.
- Postpones the problem - how do you analyze, or restart with different # of procs?



Planning your I/O

- Parallel computation, several options.
- We're going to learn to avoid doing this by using Parallel I/O
- **Coordinated** single output of multiple processes.



Where, how you do I/O matters.

- Binary - smaller files, *much* faster to read/write.
- You're not going to read GB/TB of data yourself; don't bother trying.
- Write in 1 chunk, rather than a few #s at a time.

	ASCII	binary
Large Parallel File System		
	173s	6s
Ramdisk		
	174s	1s
Typical work station disk		
	260s	20s

Timing data: writing 128M double-precision numbers

Where, how you do I/O matters.

- *All* disk systems do best when reading/writing large, contiguous chunks
- I/O operations (IOPS) are themselves expensive
- moving around within a file
- opening/closing
- Seeks - 3-15ms - enough time to read 0.75 MB!

Typical work station disk
binary - one large read 14s
binary - 8k at a time 20s
binary - 8k chunks, lots of seeks 150s
binary - seeky + open and closes 205s

Timing data: reading 128M double-precision numbers

Where, how you do I/O matters.

- RAM is much better for random accesses
- Use right storage medium for the job!
- Where possible, read in contiguous large chunks, do random access in memory
- Much better *if* you use most of data read in

Large Parallel File System

ASCII	binary
173s	6s

Ramdisk

ASCII	binary
174s	1s

Typical work station disk

ASCII	binary
260s	20s

Ramdisk

binary - one large read
1s

binary - 8k at a time
1s

binary - 8k chunks, lots of seeks
1s

binary - seeky + open and closes
1.5s

Parallel I/O and large file systems

- Large disk systems featuring many servers, disks
- Can serve files to many clients concurrently
- Parallel File Systems -
- Lustre, Panasas, GlusterFS, Ceph, GPFS...

SciNet ~2k drives

SciNet's File Systems

- 2x DCS9900 couplets
- 1,790 1TB SATA disk drives
- 1.4 PB of storage
- Single GPFS domain, accessed by all machines (TCS and GPC).
- Data to compute nodes via IB

SciNet's File Systems

- Designed for HPC workloads
- High bandwidth to large files - big data.
- Does not do well with millions of little files:
  - wastes disk space (4MB block size)
  - lots of small scattered access is *terrible* for performance, even on desktop; multiply by hundreds of processors, can be disastrous

Understanding storage performance

Device	Bandwidth (MB/s)	IOPS
SATA HDD	100	100
SSD	250	10000
SciNet GPFS	5000	30000

(SciNet GPFS used by ~3000 nodes.)

Where, how you do I/O matters.

- Well built parallel file systems can greatly increase bandwidth
- Many pipes to network (servers), many spinning disks (bandwidth off of disks)
- But typically even **worse** penalties for seeky/IOPSy operations (coordinating all those disks.)
- Parallel FS can help with big data in two ways

Large Parallel File System

ASCII	**binary**
173s	6s

Ramdisk

ASCII	**binary**
174s	1s

Typical work station disk

ASCII	**binary**
260s	20s

Large Parallel File System

binary - one large read
7.5s

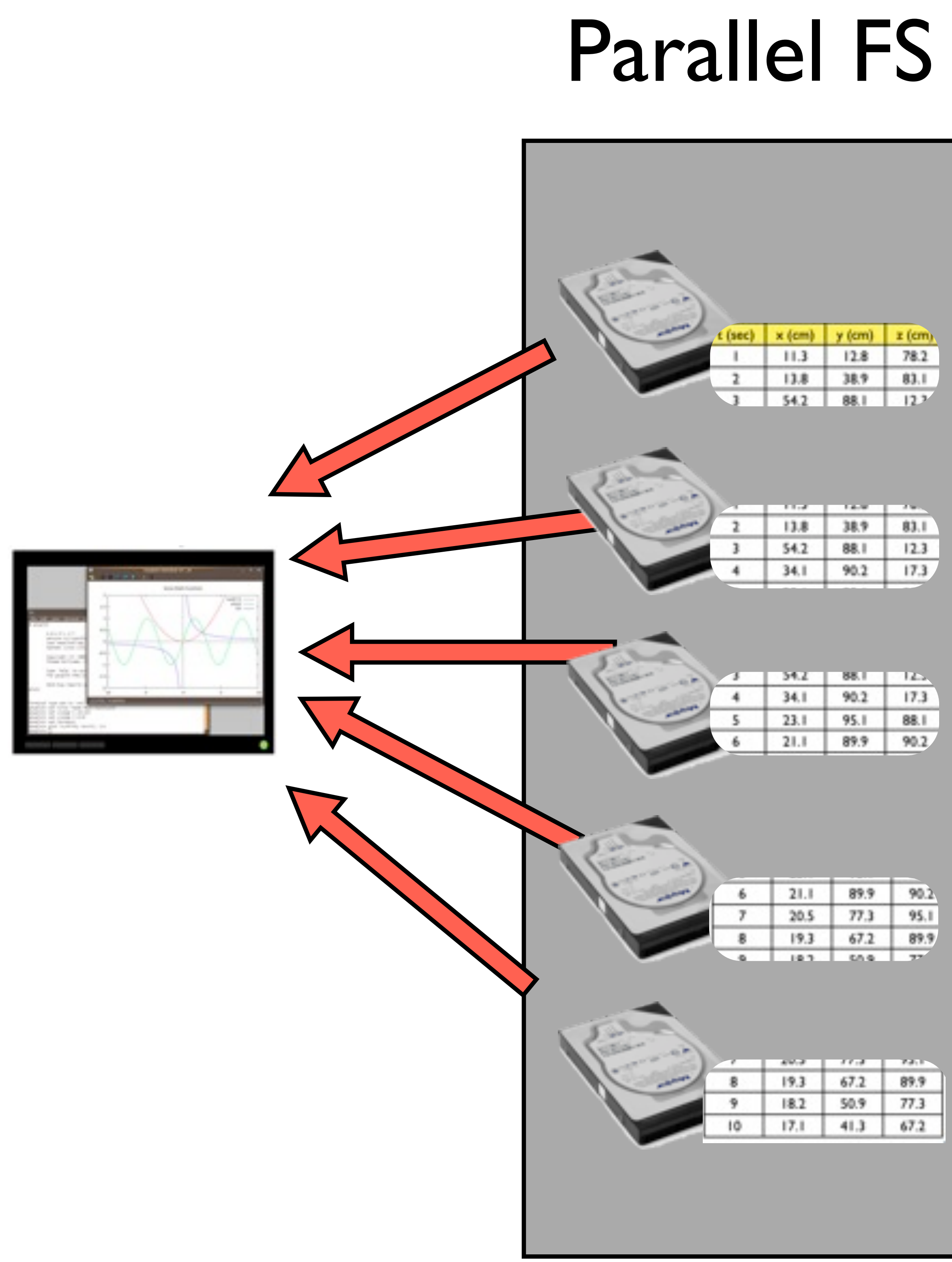
binary - 8k at a time
62 s

binary - 8k chunks, lots of seeks
428 s

binary - seeky + open and closes
2137 s

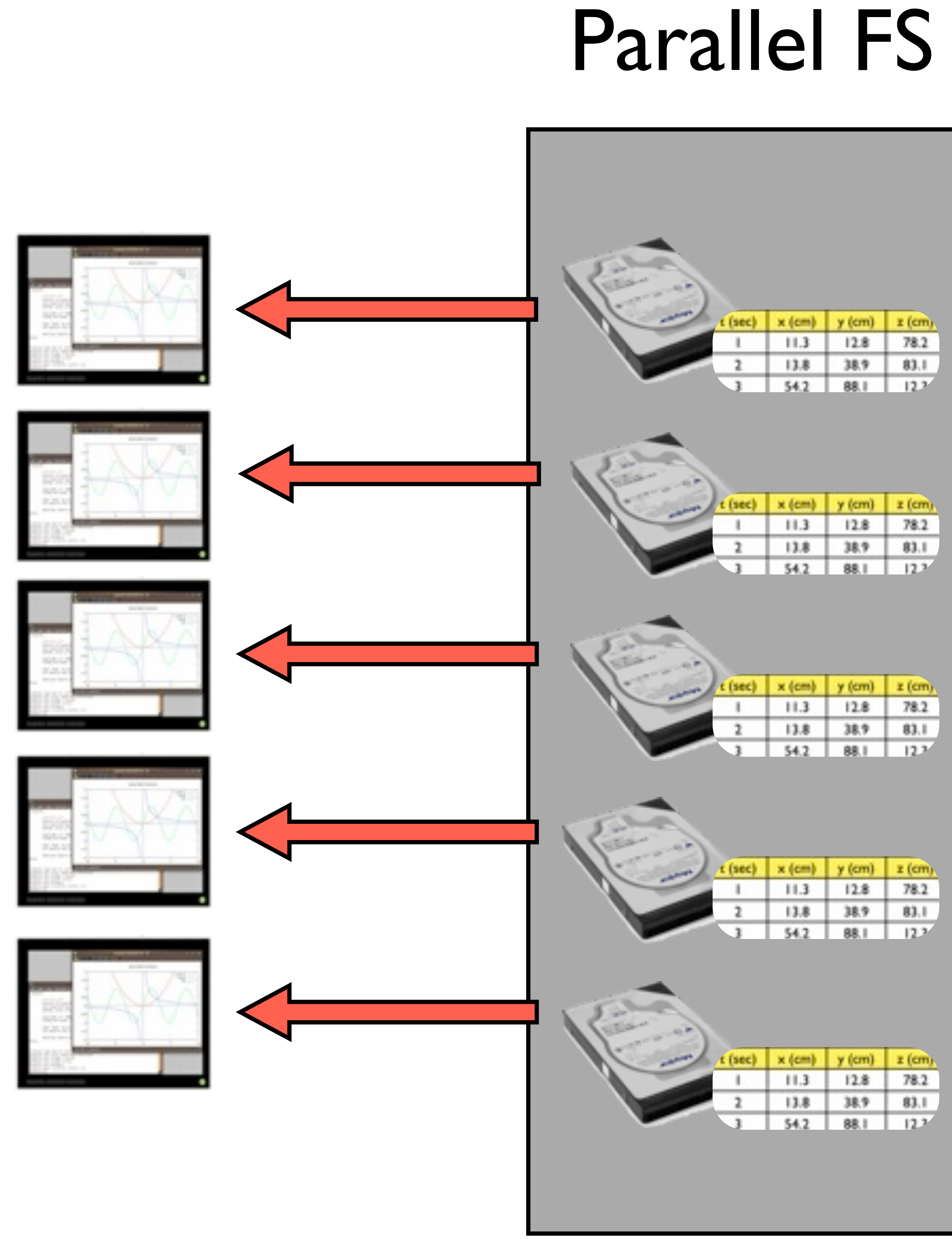
Striping data across disks

- Single client can make use of multiple disk systems simultaneously
- “Stripe” file across many drives
- One drive can be finding next block while another is sending current block



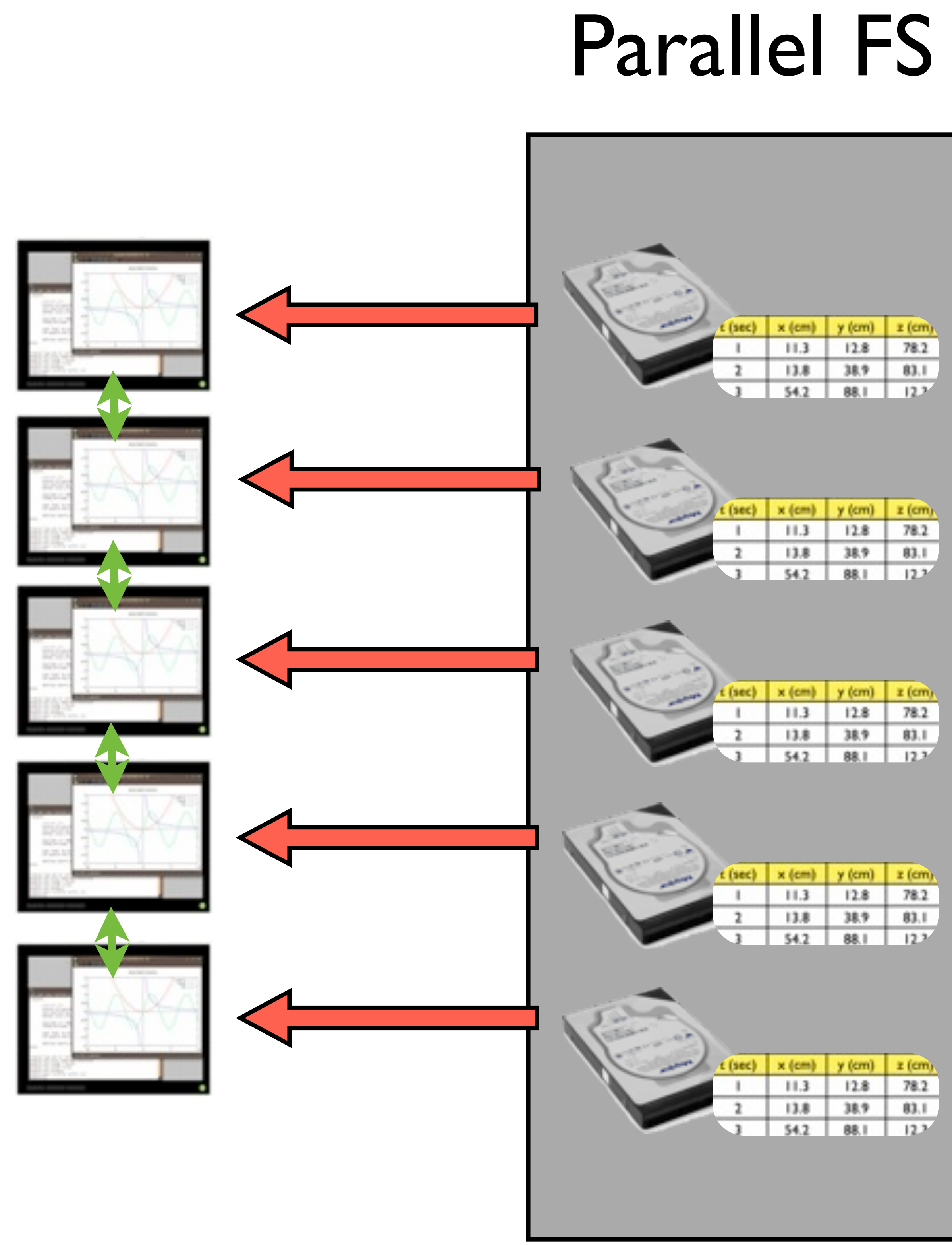
Parallel operations on separate data

- Or can do truly parallel operations
- multiple clients doing independent work
- Easy parallelism (good for lots of small data) - process many small files separately



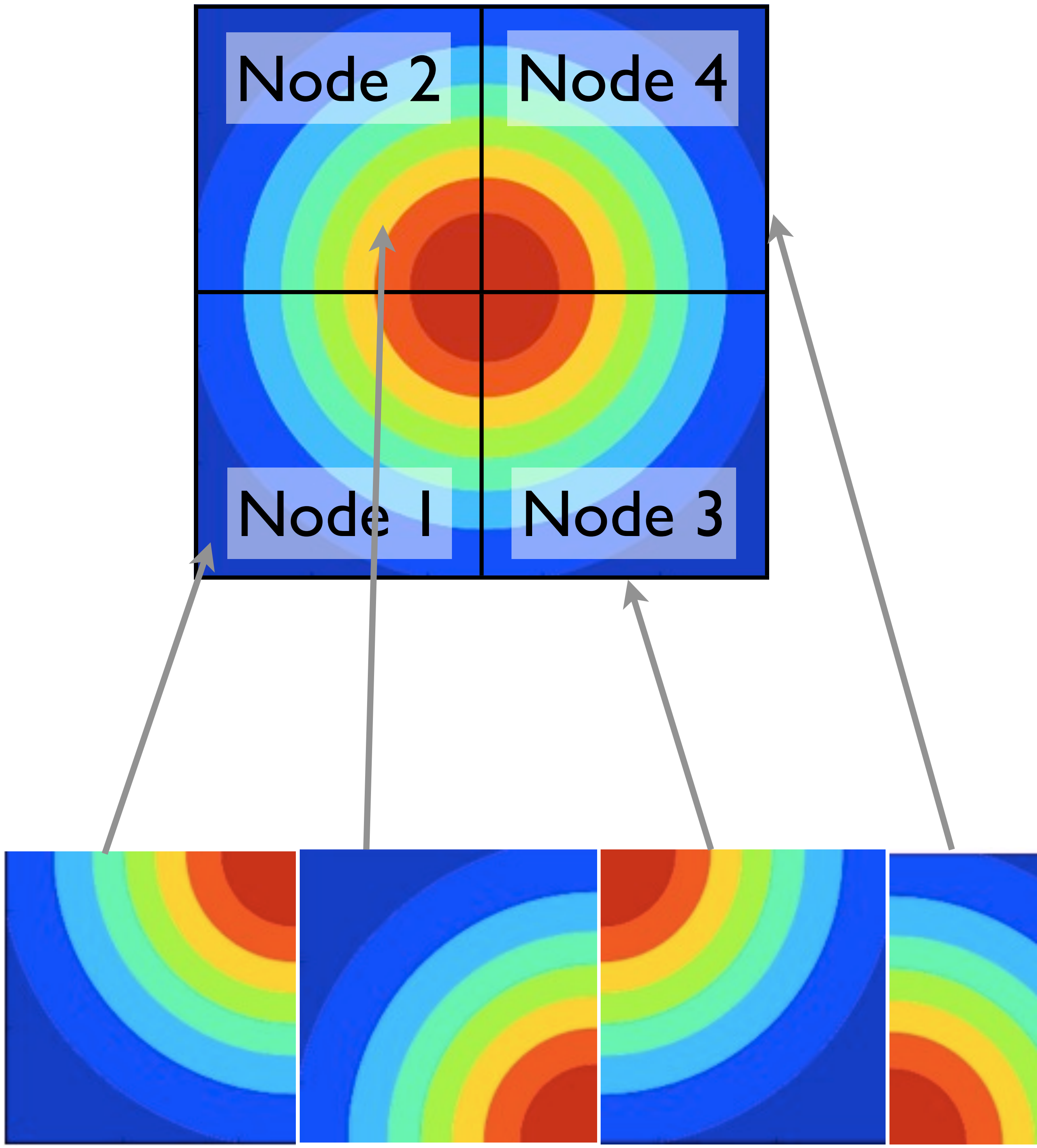
Parallel operations on separate data

- Or can do truly parallel operations
- multiple clients doing independent work
- Easy parallelism (good for lots of small data) - process many small files separately
- Harder parallelism - each does part of a larger analysis job on a big file.



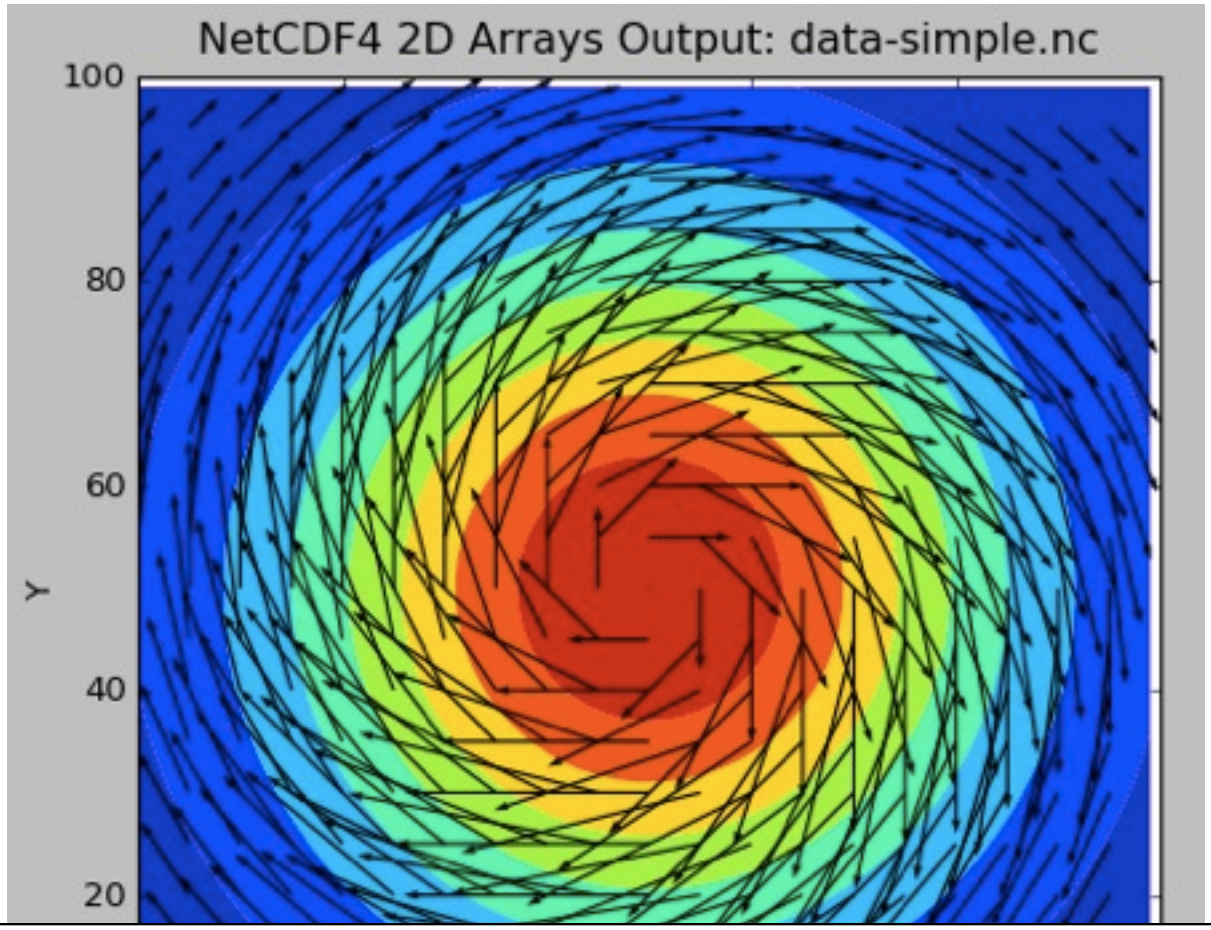
Data files must take advantage of parallel I/O

- For parallel operations on single big files, parallel filesystem isn't enough
- Data must be written in such a way that nodes can efficiently access relevant subregions
- HDF5, NetCDF formats typical examples for scientific data



Disk: (HDF5, NetCDF, pVTK..)

These formats are *self-describing*

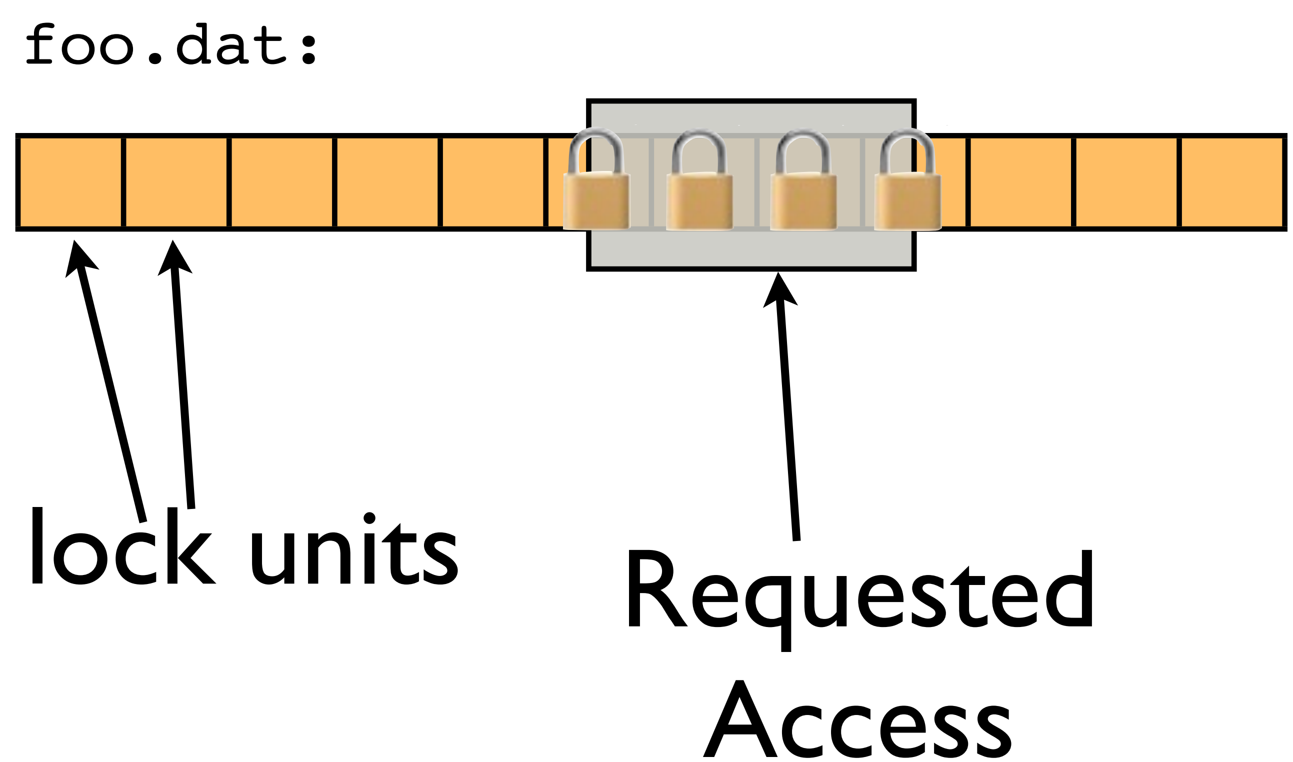


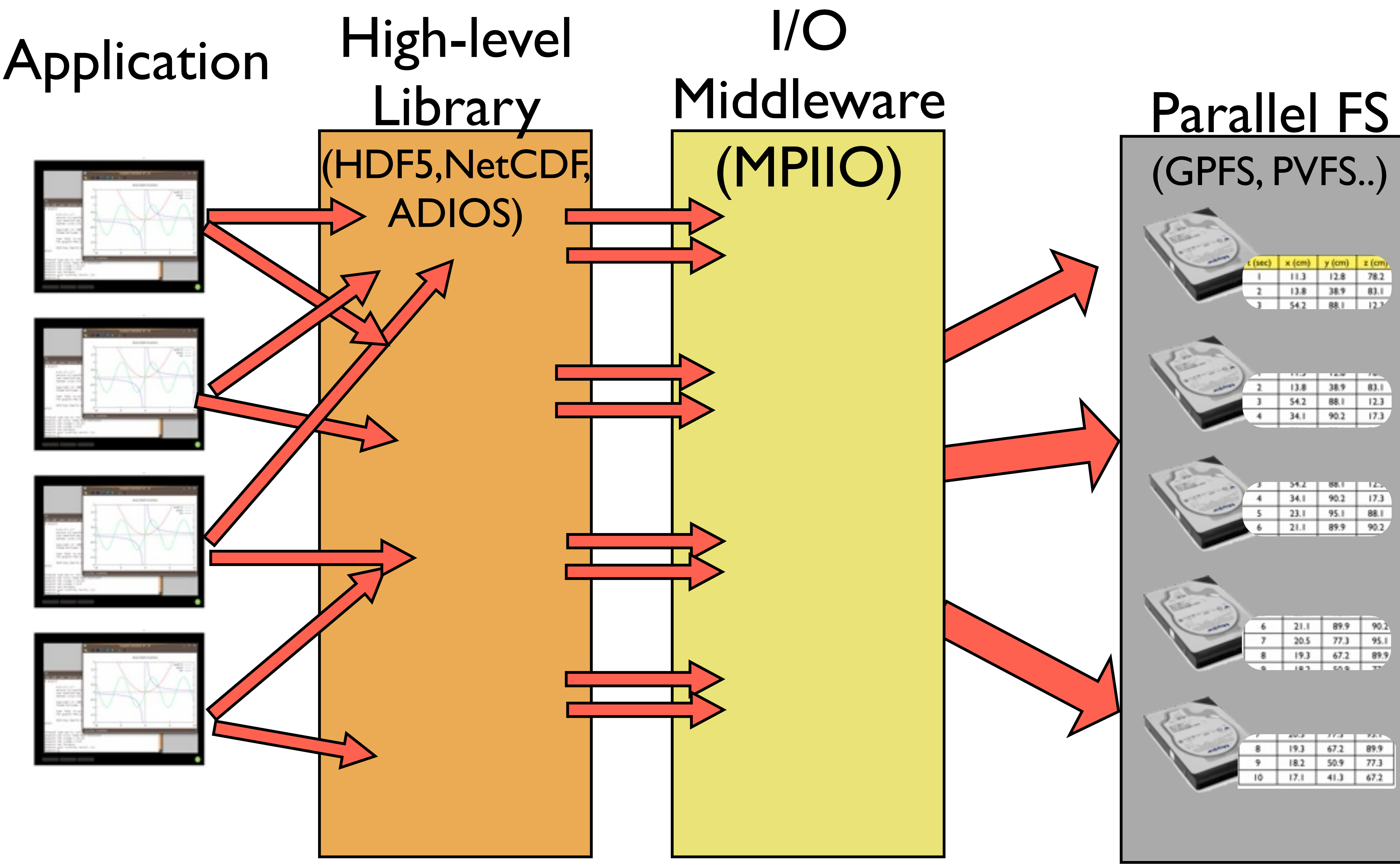
- HDF5, NetCDF have other advantages anyway
- Binary
- Self describing - contains not only data but names, descriptions of arrays, etc
- Many tools can read these formats
- Big data - formats matter

```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity components = 2 ;
variables:
   double Density(Y, X) ;
   double Velocity(Y, X, velocity components) ;
}
```

Coordinating I/O

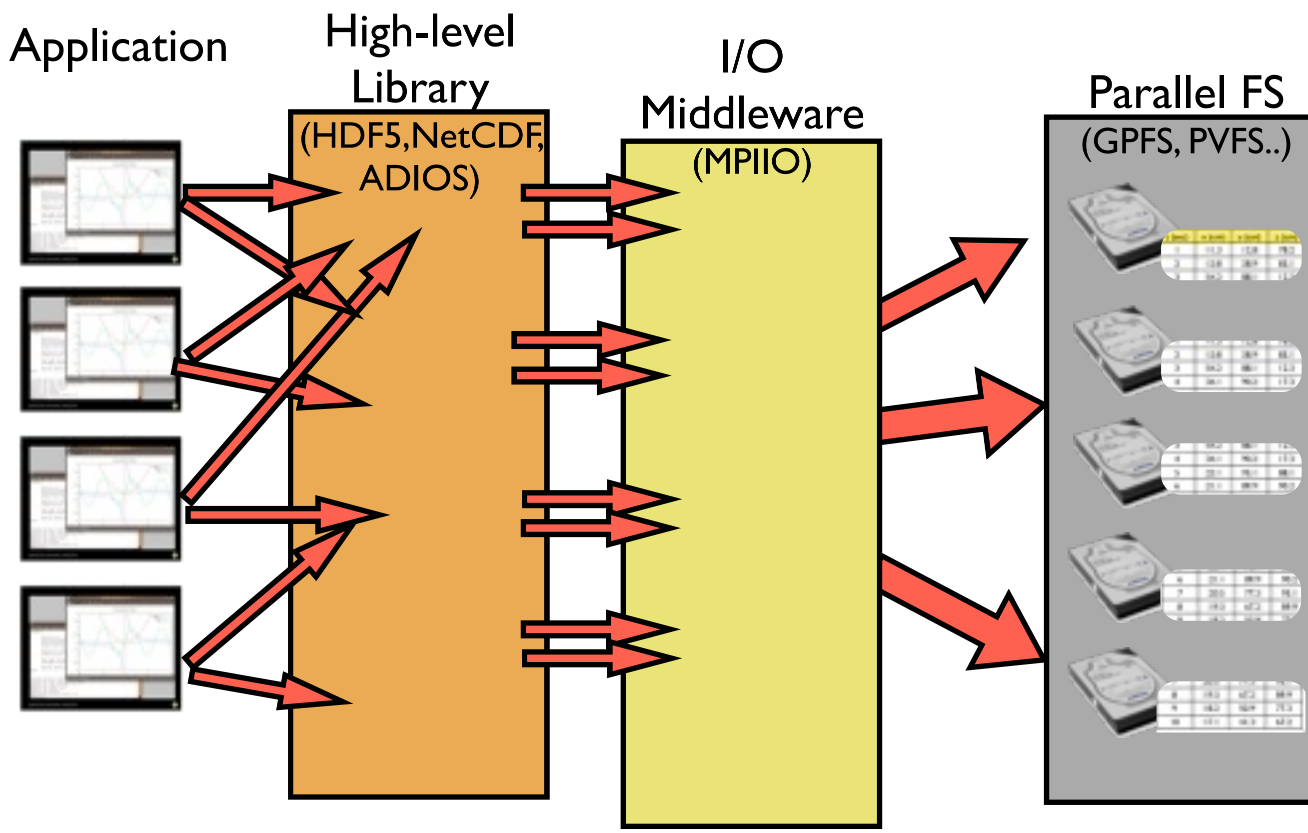
- Multiple nodes all accessing same filesystem.
- To prevent anarchy, locks for some requested accesses.
- File broken up into lock units, locks handed out upon request.
- “False sharing”, etc, possible.
- Files **and** directories.
- Makes (some) IOPS even more expensive




Application
High-level Library
(HDF5,NetCDF, ADIOS)
I/O Middleware
(MPIIO)
Parallel FS
(GPFS, PVFS..)

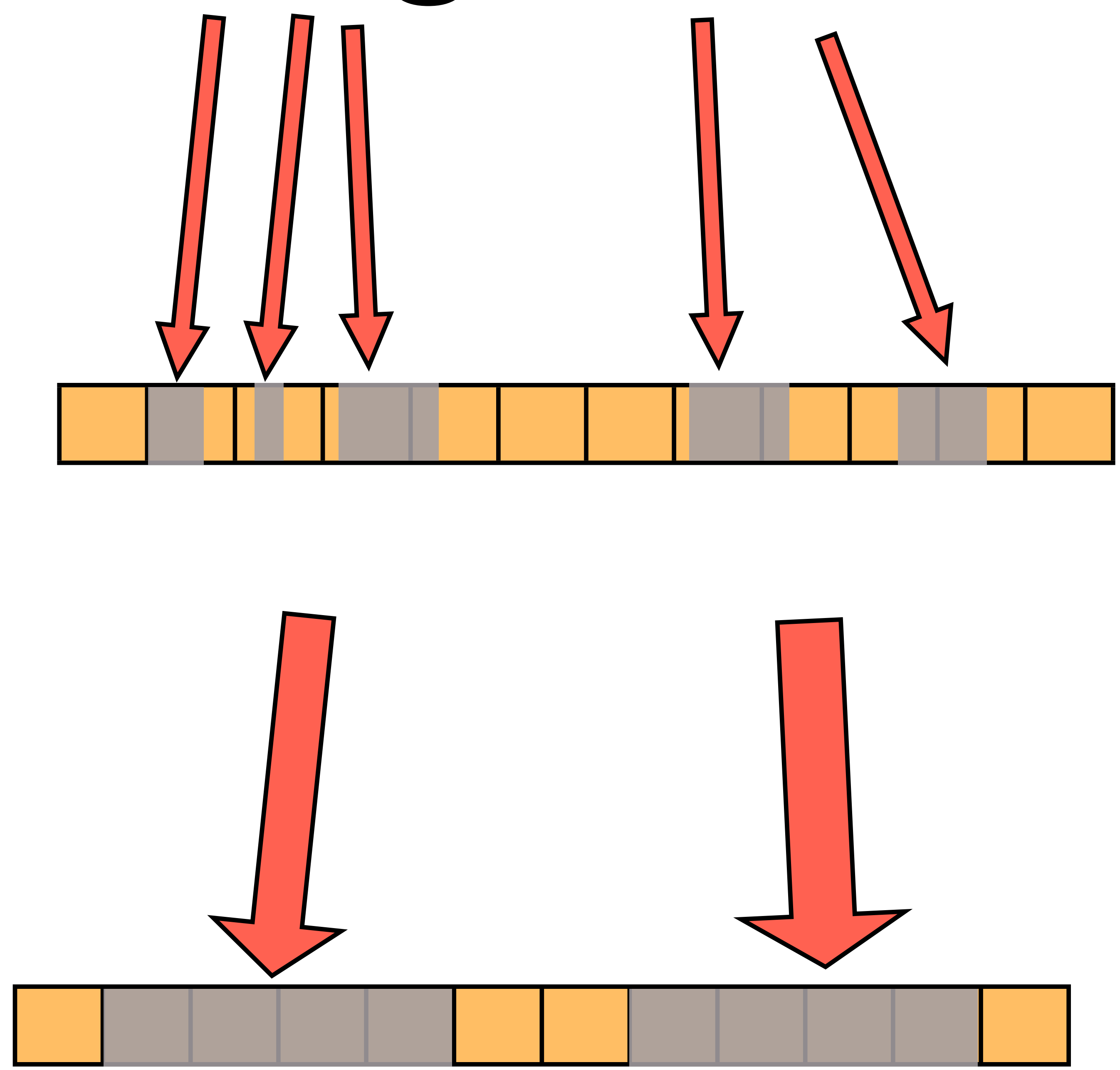
Abstraction Layers

- High Level libraries can simplify programmers tasks
  - Express IO in terms of the data structures of the code, not bytes and blocks
- I/O middleware can coordinate, improve performance
  - Data Sieving
  - 2-phase I/O



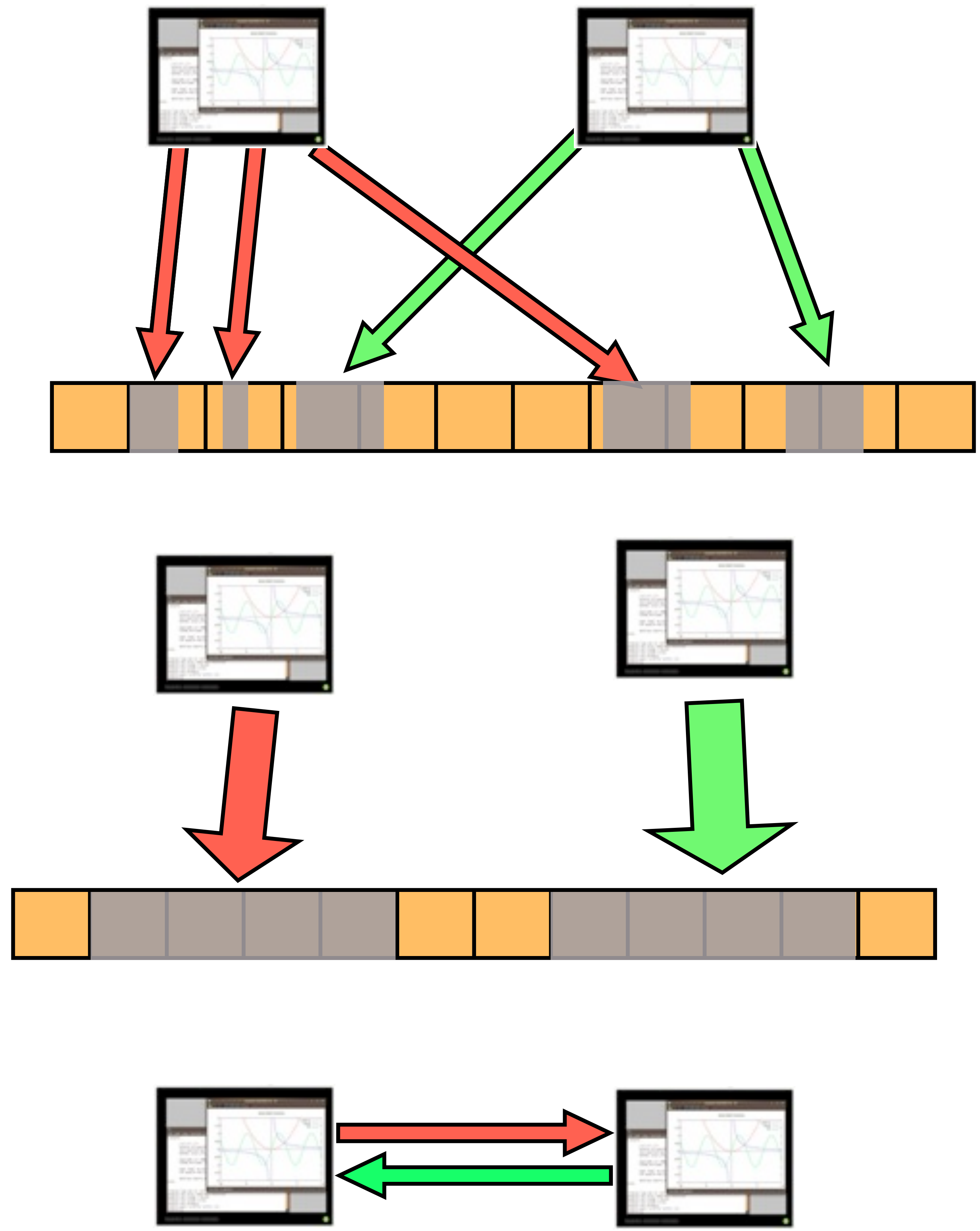
Data Sieving

- Combine many non-contiguous IO requests into fewer, bigger IO requests
- "Sieve" unwanted data out
- Reduces IOPS, makes use of high bandwidth for sequential IO



Two-Phase IO

- Collect requests into larger chunks
- Have individual nodes read big blocks
- Then use network communications to exchange pieces
- Fewer IOPS, faster IO
- Network communication usually faster



MPI-IO

- Part of MPI-2 standard
- Started at IBM Watson
- Maps I/O reads and writes to message passing
- ROMIO is the implementation found in MPICH2, OpenMPI
- Really only widely-available scientific computing parallel I/O middleware

```
$ cd parIO
$ source parallellibs
$ cd samples/mpiio
$ make
....

$ mpiexec -n 4 ./helloworldc
Rank 0 has message <Hello >
Rank 1 has message <World!>
Rank 2 has message <Hello >
Rank 3 has message <World!>
Rank 4 has message <Hello >

$ cat helloworld.txt
Hello World!Hello World! $
```

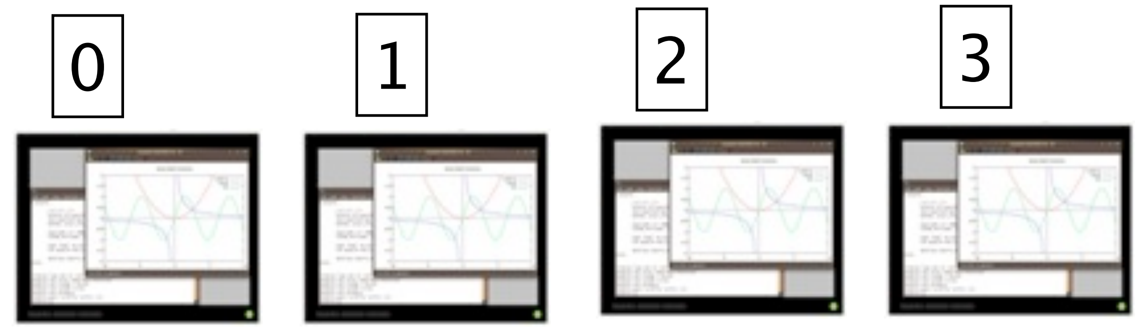
helloworldc.c

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>

int main(int argc, char **argv) {
    int ierr, rank, size;
    MPI_Offset offset;
    MPI_File   file;
    MPI_Status status;
    const int msgsize=6;
    char message[msgsize+1];

    ierr = MPI_Init(&argc, &argv);
    ierr|= MPI_Comm_size(MPI_COMM_WORLD, &size);
    ierr|= MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    if ((rank % 2) == 0) strcpy (message, "Hello "); else strcpy (message, "World!");

    offset = (msgsize*rank);

    MPI_File_open(MPI_COMM_WORLD, "helloworld.txt", MPI_MODE_CREATE|MPI_MODE_WRONLY,
                  MPI_INFO_NULL, &file);
    MPI_File_seek(file, offset, MPI_SEEK_SET);
    MPI_File_write(file, message, msgsize, MPI_CHAR, &status);
    MPI_File_close(&file);

    MPI_Finalize();
    return 0;
}
```

helloworldf.f90

```fortran
program MPIIO_helloworld
    use mpi
    implicit none

    integer(mpi_offset_kind) :: offset
    integer, dimension(mpi_status_size) :: wstatus
    integer, parameter :: msgsize=6
    character(msgsize) :: message
    integer :: ierr, rank, comsize, fileno

    call MPI_Init(ierr)
    call MPI_Comm_size(MPI_COMM_WORLD, comsize, ierr)
    call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)

    if (mod(rank,2) == 0) then
        message = "Hello "
    else
        message = "World!"
    endif

    offset = rank*msgsize

    call MPI_File_open(MPI_COMM_WORLD, "helloworld.txt", ior(MPI_MODE_CREATE,MPI_MODE_WRONLY),&
                       MPI_INFO_NULL, fileno, ierr)
    call MPI_File_seek (fileno, offset, MPI_SEEK_SET, ierr)
    call MPI_File_write(fileno, message, msgsize, MPI_CHARACTER, wstatus, ierr)
    call MPI_File_close(fileno, ierr)

    call MPI_Finalize(ierr)

end program MPIIO_helloworld
```

MPI-IO Hello World

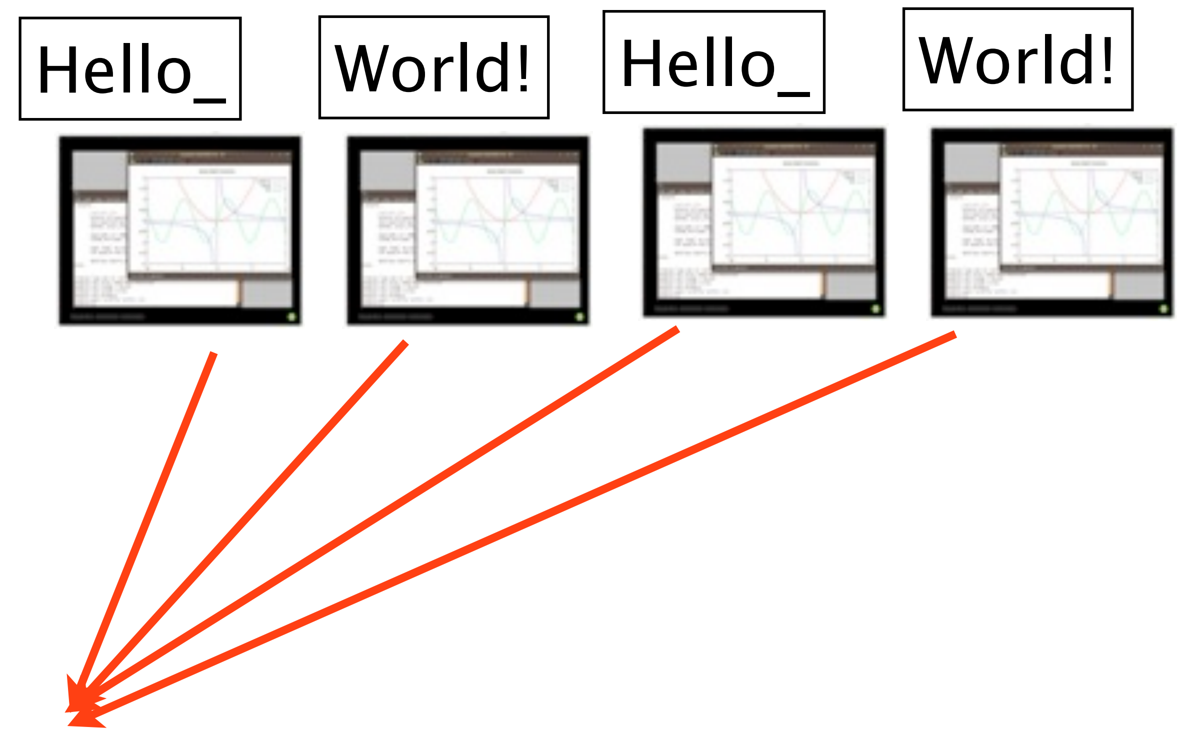



```
mpiexec -n 4 ./helloworldc
```

MPI-IO Hello World


```
if ((rank % 2) == 0)
  strcpy (message, "Hello ");
else
  strcpy (message, "World!");
```

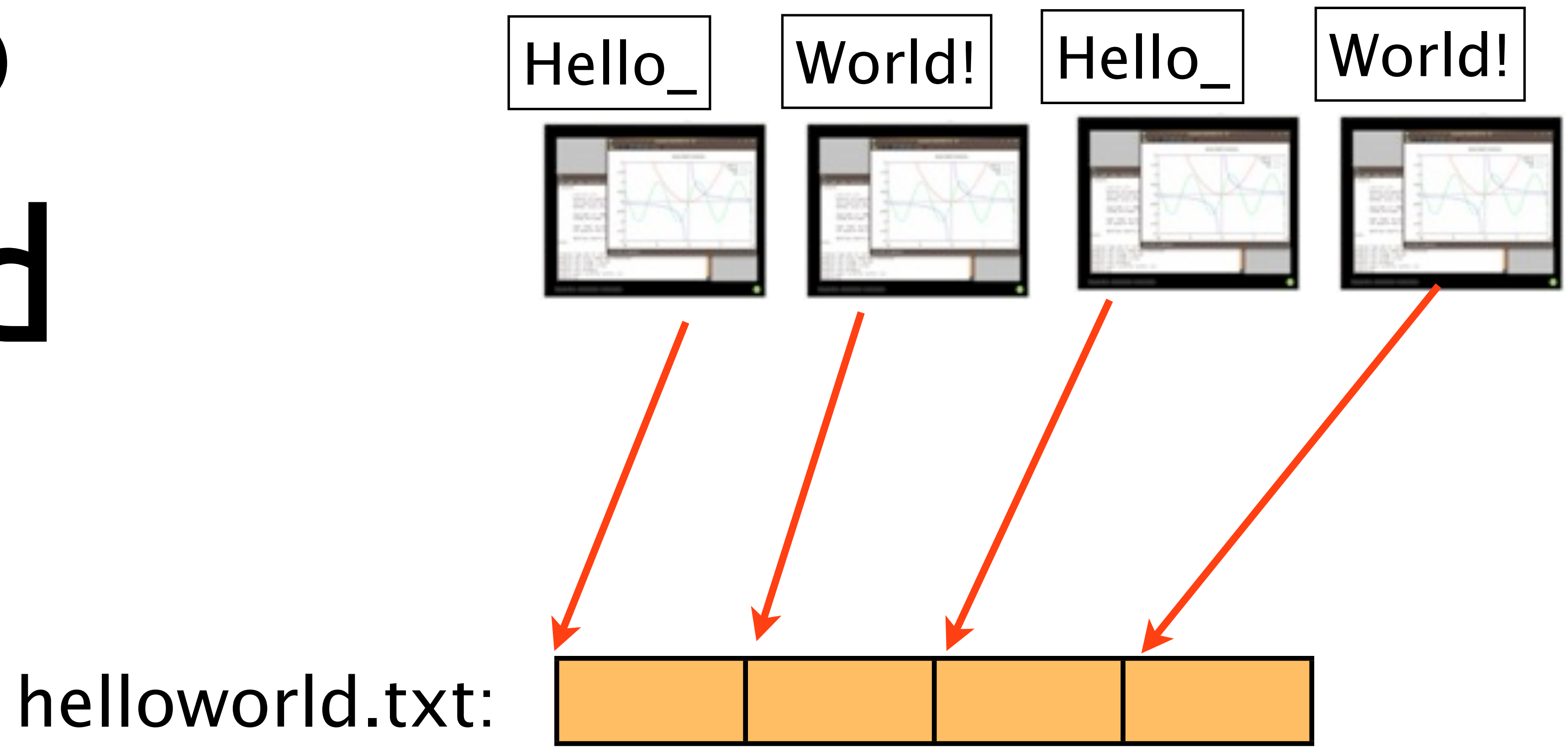
MPI-IO Hello World



helloworld.txt:

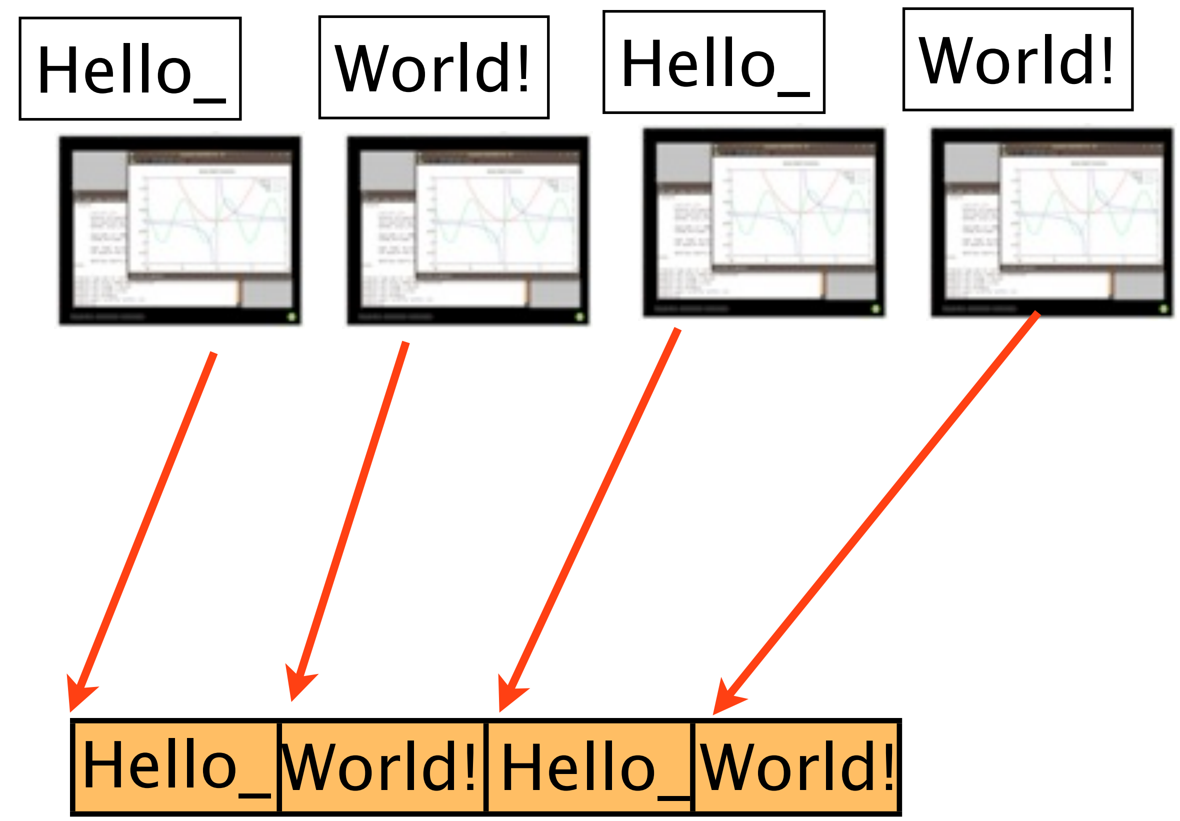
```
MPI_File_open(MPI_COMM_WORLD, "helloworld.txt", MPI_MODE_CREATE|MPI_MODE_WRONLY,
                  MPI_INFO_NULL, &file);
```

MPI-IO Hello World




```
offset = (msgsize*rank);

MPI_File_seek(file, offset, MPI_SEEK_SET);
```

MPI-IO Hello World



helloworld.txt:

```
MPI_File_write(file, message, msgsize, MPI_CHAR, &status);
```

MPI-IO Hello World

helloworld.txt: | Hello_ | World! | Hello_ | World! |

```
MPI_File_close(&file);
```

MPI-IO Hello World

Usual MPI startup/ teardown boilerplate

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>

int main(int argc, char **argv) {
    int ierr, rank, size;
    MPI_Offset offset;
    MPI_File   file;
    MPI_Status status;
    const int msgsize=6;
    char message[msgsize+1];

    ierr = MPI_Init(&argc, &argv);
    ierr|= MPI_Comm_size(MPI_COMM_WORLD, &size);
    ierr|= MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    if ((rank % 2) == 0) strcpy (message, "Hello "); else strcpy (me

    offset = (msgsize*rank);

    MPI_File_open(MPI_COMM_WORLD, "helloworld.txt", MPI_MODE_CREATE
                  MPI_INFO_NULL, &file);
    MPI_File_seek(file, offset, MPI_SEEK_SET);
    MPI_File_write(file, message, msgsize, MPI_CHAR, &status);
    MPI_File_close(&file);

    MPI_Finalize();
    return 0;
}
```

MPI_File_Open

Communicator;
collective
operation.

```
call MPI_File_Open( integer       communicator,
                    character(*) *filename,
                    integer       mode,
                    integer       info,
                    integer       handle,
                    integer       ierr);
```

```
int MPI_File_Open( MPI_Comm  communicator,
                   char     *filename,
                   int       mode,
                   MPI_Info  info,
                   MPI_File *handle);
```

MPI_File_Open

Info allows us to send extra hints to MPI-IO layer about file(performance tuning, special case handling)

MPI_INFO_NULL: no extra info.

```
call MPI_File_Open( integer          communicator,
                    character(*)   *filename,
                    integer          mode,
                    integer          info,
                    integer          handle,
                    integer          ierr);
```

```
int MPI_File_Open( MPI_Comm   communicator,
                   char      *filename,
                   int        mode,
                   MPI_Info   info,
                   MPI_File  *handle);
```

Modes for MPI_File_Open():

MPI_MODE_RDONLY	read-only
MPI_MODE_RDWR	read-write
MPI_MODE_WRONLY	write-only
MPI_MODE_CREATE	Create if doesn't exist.
MPI_MODE_APPEND	On open, file pointers at end of file.
MPI_MODE_EXCL	Fail if try to create, does exist.
MPI_MODE_UNIQUE_OPEN	No one else is using this.
MPI_MODE_SEQUENTIAL	Will be sequential access only.
MPI_MODE_DELETE_ON_CLOSE	Delete when done. (OOC/scratch).

MPI_File_Seek:

```
int MPI_File_seek( MPI_File mpi_fh,
                   MPI_Offset offset,
                   int mode);
```

```
call MPI_File_seek( integer :: mpi_fh,
                    integer(mpi_offset_kind) :: offset,
                    integer :: mode
                    integer :: ierr)
```

MPI_SEEK_SET	Set file pointer to position *offset*
MPI_SEEK_CUR	pointer ← current position + *offset*
MPI_SEEK_END	pointer ← end of file - *offset*

Not collective; each adjusts its own local file pointer

MPI_File_write:

```
int MPI_File_write(MPI_File fh,
                   void *buf,
                   int count,
                   MPI_Datatype datatype,
                   MPI_Status *status)
```

```
call MPI_File_write( integer :: mpi_fh,
                     buffer,
                     integer :: count
                     integer :: datatype
                     integer :: status(MPI_STATUS_SIZE)
                     integer :: ierr)
```

Not collective; each writes.

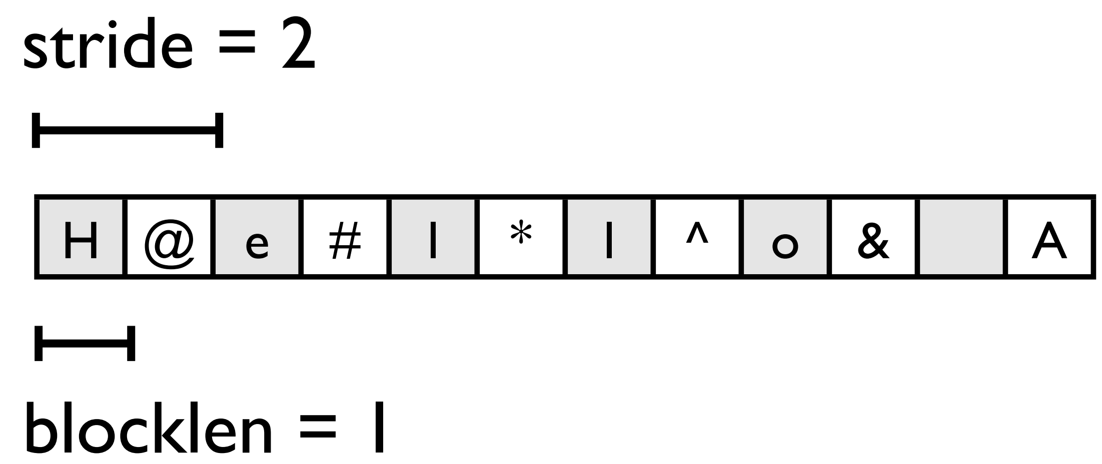
MPI_File_write:

- MPI File write is very much like a MPI_Send.
- "Sending" count of datatype from buf "to" the file.
- Here, writing 6 MPI_CHARs.
- Contiguous in memory starting in buffer.
- Status like a receive -- contains info about amount of data actually written, etc.

```
int MPI_File_write(MPI_File fh,
                   void *buf,
                   int count,
                   MPI_Datatype datatype,
                   MPI_Status *status)
```

MPI_File_write:

- To write out data that is non-contiguous in memory, same as MPI_Sending non-contig data:
  - Create type that describes data layout in memory
  - “Send” in units of that type.
- Noncontiguous data in memory is written out contiguously to the file, starting at the current (local) file pointer.



count = 6

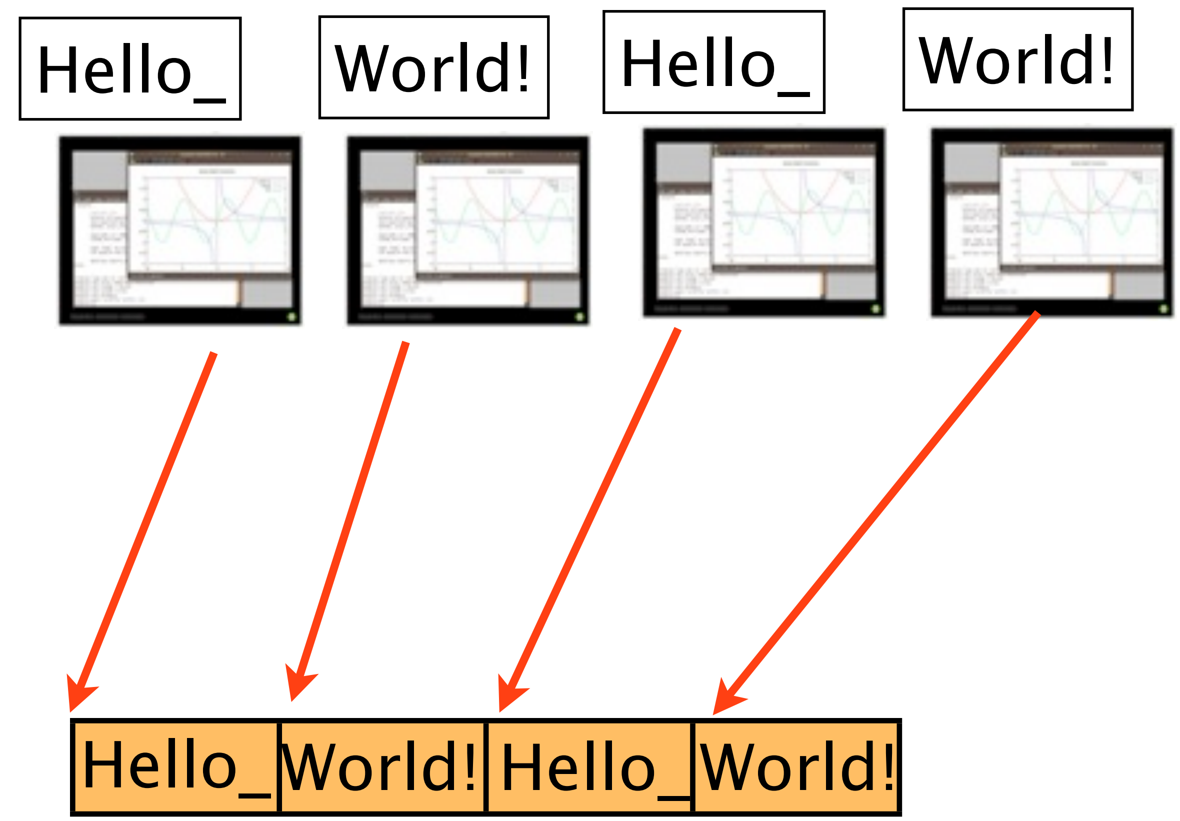
```
call MPI_Type_vector(count, blocklen, stride,
                     MPI_CHARACTER,
                     everyother, ierr)
```

helloworld-noncontigf.f90

```
integer, parameter :: msgsize=6, strsize=12
character(strsize) :: message
integer :: everyother

!....

if (mod(rank,2) == 0) then
    message = "H@e#l*l^o* A"
else
    message = "WFoQr#l>d@!_"
endif

!...

call MPI_Type_vector(msgsize, 1, 2, MPI_CHARACTER, everyother, ierr)
call MPI_Type_commit(everyother, ierr)

call MPI_File_open(MPI_COMM_WORLD, "helloworld-nc.txt", ior(MPI_MODE_CREATE,MPI_MODE_WRONLY),&
                     MPI_INFO_NULL, fileno, ierr)

call MPI_File_seek (fileno, offset, MPI_SEEK_SET, ierr)
call MPI_File_write(fileno, message, 1, everyother, wstatus, ierr)
call MPI_File_close(fileno, ierr)
```

Seek + Write

- Works, but:
  - Very low level (gets complicated for less trivial data layouts)
  - Completely independent operations (seek, write)
  - Hard for any middleware to coordinate, improve anything.
  - Could do this with POSIX I/O.



MPI_File_write_at:

writeatf.f90

```
offset = rank*msgsize

call MPI_File_open(MPI_COMM_WORLD, "helloworld-at.txt",
                   ior(MPI_MODE_CREATE,MPI_MODE_WRONLY), &
                   MPI_INFO_NULL, fileno, ierr)

call MPI_File_write_at(fileno, offset, message, msgsize, &
                    MPI_CHARACTER, wstatus, ierr)
call MPI_File_close(fileno, ierr)
```

writeatc.c

```
offset = (msgsize*rank);

MPI_File_open(MPI_COMM_WORLD, "helloworld-at.txt",
              MPI_MODE_CREATE|MPI_MODE_WRONLY,
              MPI_INFO_NULL, &file);

MPI_File_write_at(file, offset, message, msgsize, MPI_CHAR, &status);
MPI_File_close(&file);
```

MPI_File_write_at:

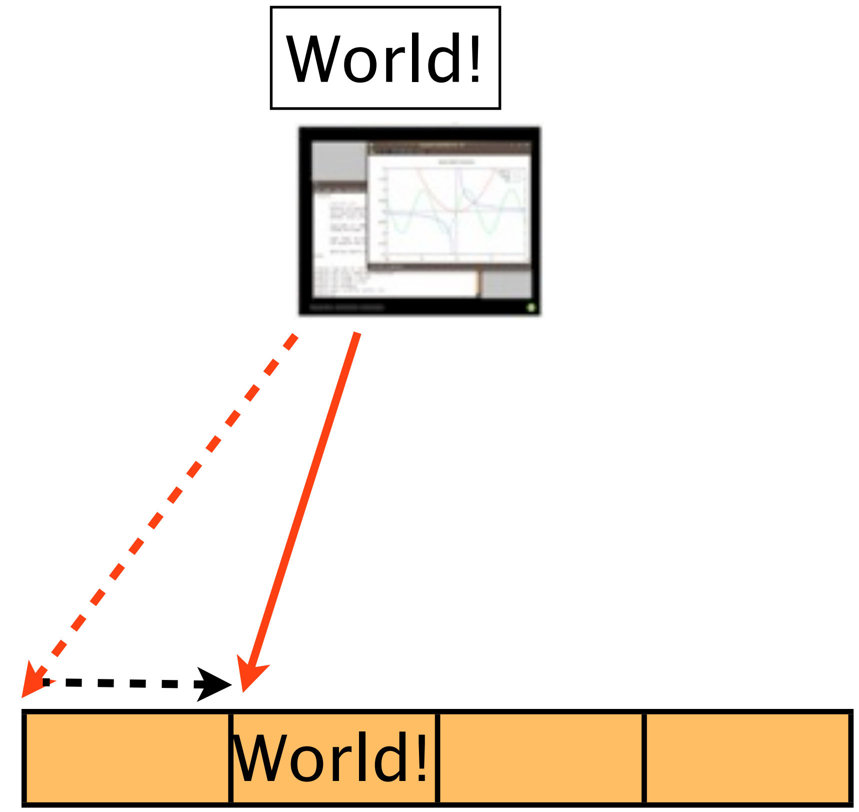
```
int MPI_File_write_at(MPI_File fh,
                      MPI_Offset offset
                      void *buf,
                      int count,
                      MPI_Datatype datatype,
                      MPI_Status *status)
```

```
call MPI_File_write_at( integer :: mpi_fh,
                        integer(MPI_OFFSET_KIND) :: offset,
                        buffer,
                        integer :: count
                        integer :: datatype
                        integer :: status(MPI_STATUS_SIZE)
                        integer :: ierr)
```

Writes at a given offset

Write_at

- Seek (relative to current, local, file pointer) + write in one operation.
- More explicit about what is going to happen - some opt. possible.
- But actions of individual processors still independent - no collective optimization possible.



MPI_File_write_at_all:

writeatallf.f90

```
offset = rank*msgsize

call MPI_File_open(MPI_COMM_WORLD, "helloworld-at.txt",   &
                   ior(MPI_MODE_CREATE,MPI_MODE_WRONLY), &
                   MPI_INFO_NULL, fileno, ierr)

call MPI_File_write_at_all(fileno, offset, message, msgsize, &
                           MPI_CHARACTER, wstatus, ierr)
call MPI_File_close(fileno, ierr)
```

writeatallc.c

```
offset = (msgsize*rank);

MPI_File_open(MPI_COMM_WORLD, "helloworld-at.txt",
              MPI_MODE_CREATE|MPI_MODE_WRONLY,
              MPI_INFO_NULL, &file);

MPI_File_write_at_all(file, offset, message, msgsize,
                      MPI_CHAR, &status);
MPI_File_close(&file);
```

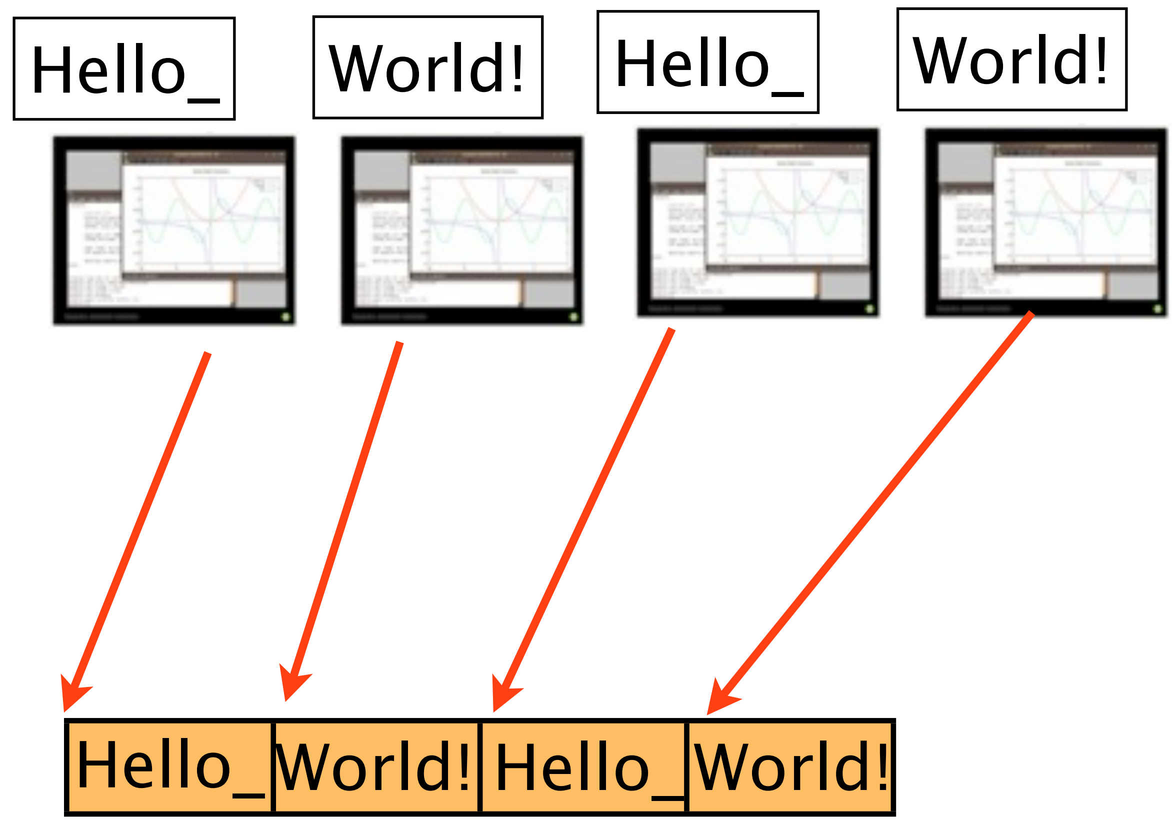
MPI_File_write_at_all:

```
int MPI_File_write_at_all(MPI_File fh,
                          MPI_Offset offset
                          void *buf,
                          int count,
                          MPI_Datatype datatype,
                          MPI_Status *status)
```

```
call MPI_File_write_at_all( integer :: mpi_fh,
                            integer(MPI_OFFSET_KIND) :: offset,
                            buffer,
                            integer :: count
                            integer :: datatype
                            integer :: status(MPI_STATUS_SIZE)
                            integer :: ierr)
```

Writes at a given offset - Collective!

Write_at_all



- Much more explicit about what is going to happen globally.
- Collective operation.
- All processors participate.
- Higher order optimizations possible.

Non-contiguous in file

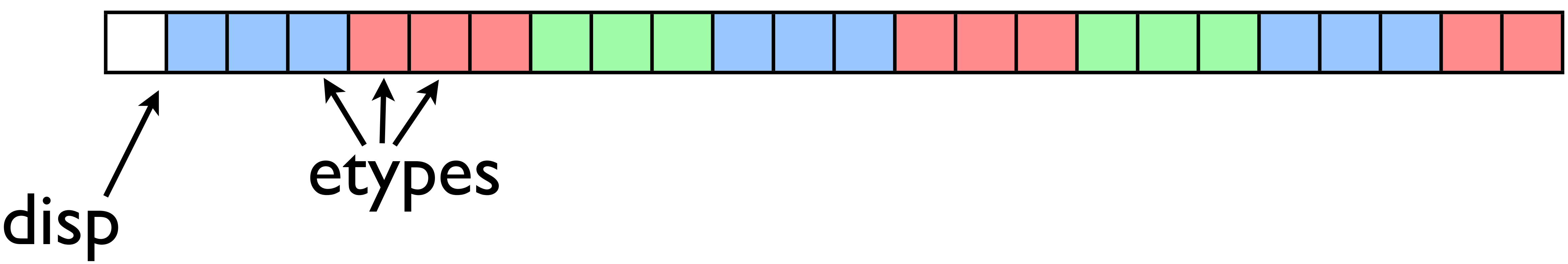
- Imagine having to write out a 2d file as to the right, with rank 0 “owning” the yellow data, etc.
- (eg, an image, or a complete checkpoint of a 2d domain).
- Would have to do repeated seeks, writing out one row at a time...

0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3

MPI-IO File View

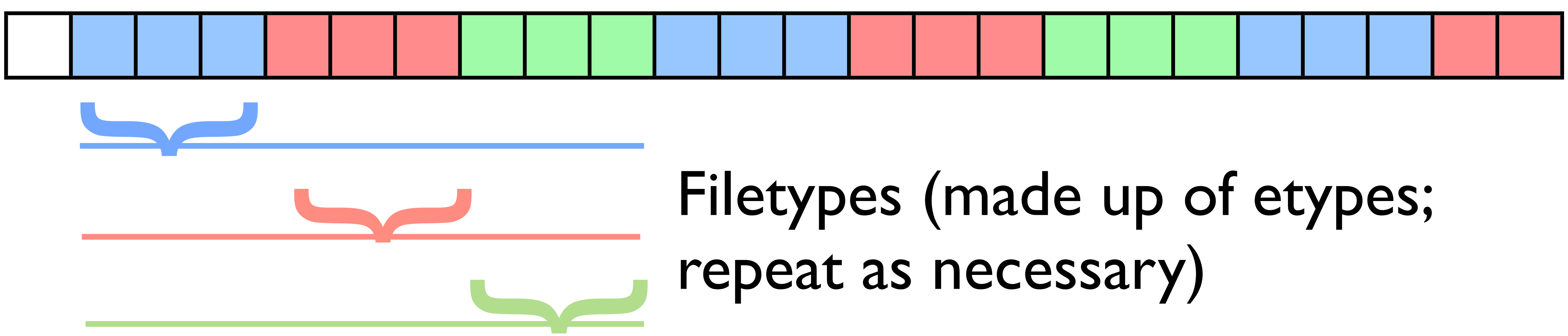
- int MPI_File_set_view(

```
MPI_File fh,                  /* displacement in bytes from start */
MPI_Offset disp,              /* elementary type */
MPI_Datatype etype,           /* file type; prob different for each proc */
MPI_Datatype filetype,        /* 'native' or 'internal' */
char *datarep,                /* MPI_INFO_NULL */
MPI_Info info)
```



MPI-IO File View

- int MPI_File_set_view(
  MPI_File fh, /* displacement in *bytes* from start */
  MPI_Offset disp, /* elementary type */
  MPI_Datatype etype, /* file type; prob different for each proc */
  MPI_Datatype filetype, /* 'native' or 'internal' */
  char *datarep, /* MPI_INFO_NULL */
  MPI_Info info)



Filetypes (made up of etypes; repeat as necessary)

MPI-IO File Write

- int MPI_File_write_all(
    MPI_File fh,
    void *buf,
    int count,
    MPI_Datatype datatype,
    MPI_Status *status)

Writes (_all: collectively) to part of file **within view.**

MPI_Type_create _subarray

0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
0	0	0	0	0	1	1	1	1	1
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3
2	2	2	2	2	3	3	3	3	3

- MPI_Type_create_subarray ; piece of a multi-dimensional array.
- *Much* more convenient for higher-dimensional arrays
- (Otherwise, need vectors of vectors of vectors...)
- Here - starts = [0,0], subsizes=[5,5], sizes=[10,10].

```
int MPI_Type_create_subarray(
      int ndims, int *array_of_sizes,
      int *array_of_subsizes,
      int *array_of_starts,
      int order,
      MPI_Datatype oldtype,
      MPI_Datatype &newtype);

call MPI_Type_create_subarray(
      integer ndims, [array_of_sizes],
      [array_of_subsizes],
      [array_of_starts],
      order, oldtype,
      newtype, ierr)
```

fileviewc.c

```
MPI_Type_create_subarray(2, globalsize, subsize, start, MPI_ORDER_C,
                         MPI_CHAR, &viewtype);
MPI_Type_commit(&viewtype);

offset = 0;

MPI_File_open(MPI_COMM_WORLD, "viewtype.txt",
              MPI_MODE_CREATE|MPI_MODE_WRONLY,
              MPI_INFO_NULL, &file);

MPI_File_set_view(file, offset,  MPI_CHAR, viewtype,
                  "native", MPI_INFO_NULL);

MPI_File_write_all(file, &(mydata[0][0]), locnrows*locncols, MPI_CHAR, &status);
MPI_File_close(&file);
```

write locnrows*locncols contiguous MPI_CHARs to the (non-contiguous) view in file.

MPI-IO hands-on

- Fill in the blanks in sine.c or sinef.f90 to use MPI-IO to write out the 1-d array of sin(x).
- Already written: decomposing the array, doing the calculation, MPI_File_open and MPI_file_close calls.
- Make sine (sinf) and make sineplot (sinefplot) to build the code, and run it and plot the results.
- Can use any of the approaches above
- ~15 minutes.

Formats for Scientific Data Management

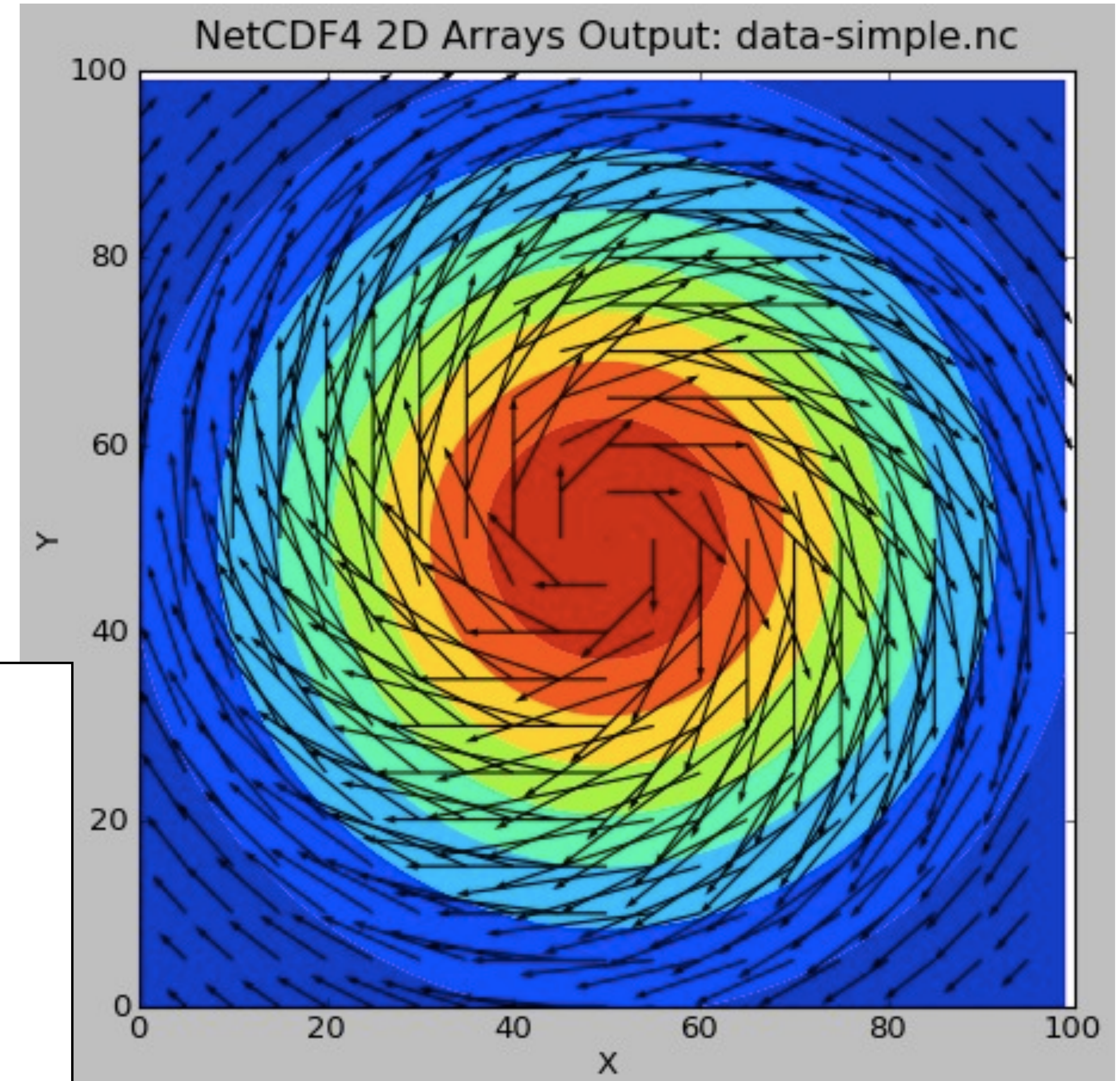
NetCDF4, HDF5, and whatnot

HPCS2012

SciNet

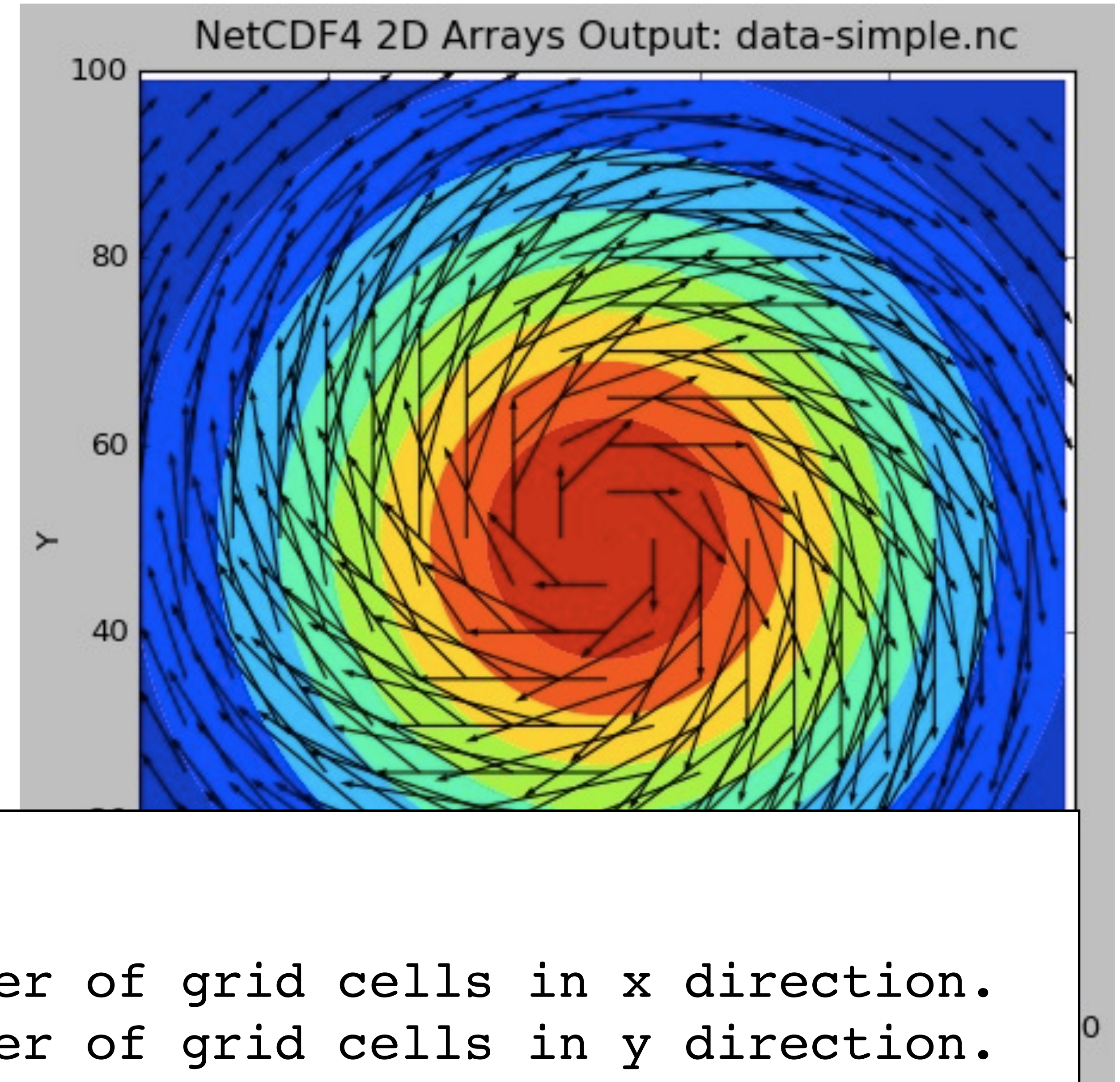
compute • calcul CANADA

Sample Code



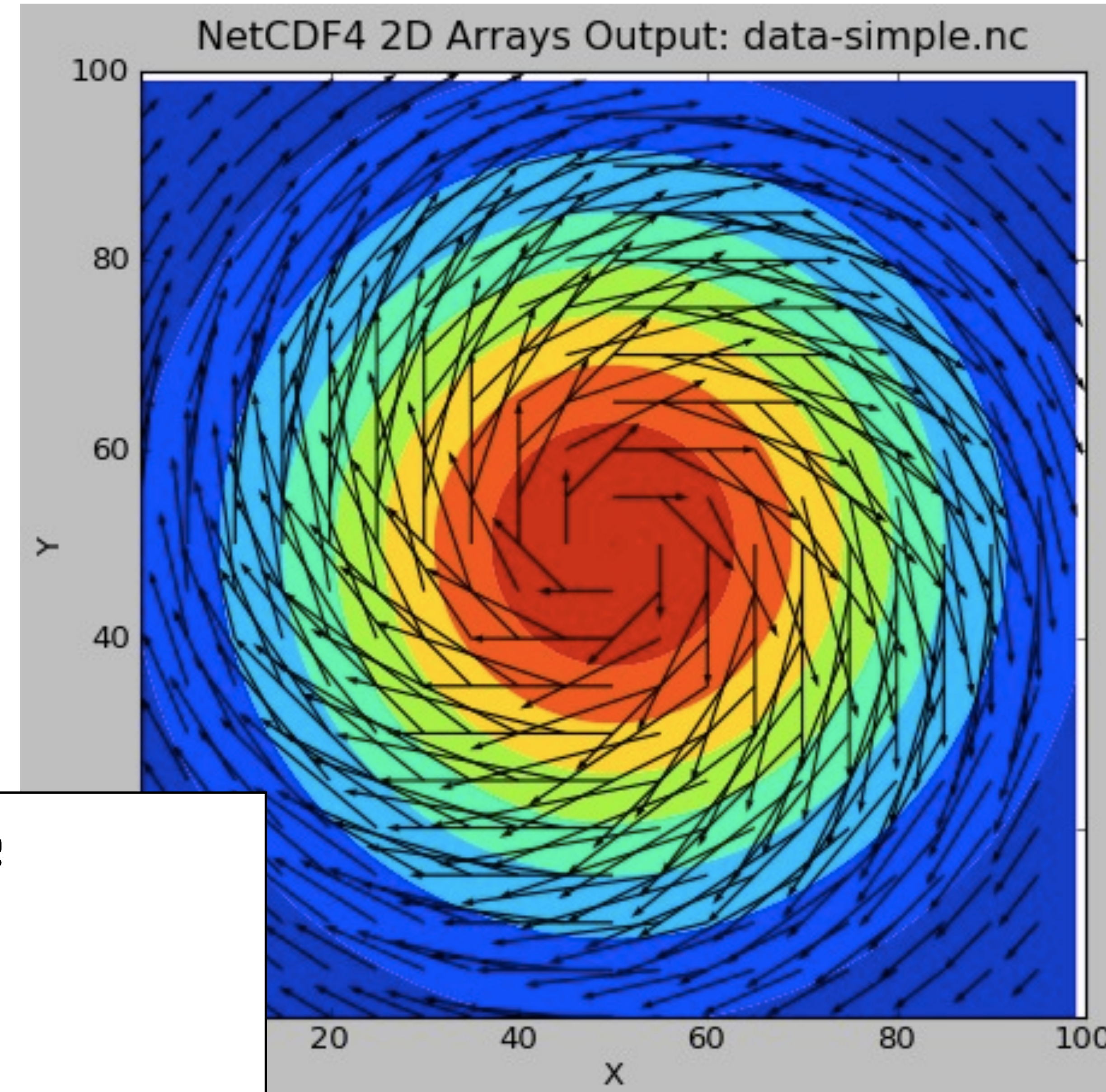

```
$ cd parIO/netcdf

$ make 2darray-simple (C), or
$ make f2darray-simple (F90)

$ ./{f,}2darray-simple

$ ls *.nc
$ ../plots.py *.nc
```

Sample Code




```
$ ./2darray-simple --help
Options:
    --nx=N          (-x N): Set the number of grid cells in x direction.
    --ny=N          (-y N): Set the number of grid cells in y direction.
    --filename=S    (-f S): Set the output filename.

$ ./f2darray-simple --help
 Usage: f2darray-simple [--help] [filename [nx [ny]]]
        where filename is output filename, and
        nx, ny are number of points in x and y directions.
```

What is this .nc file?

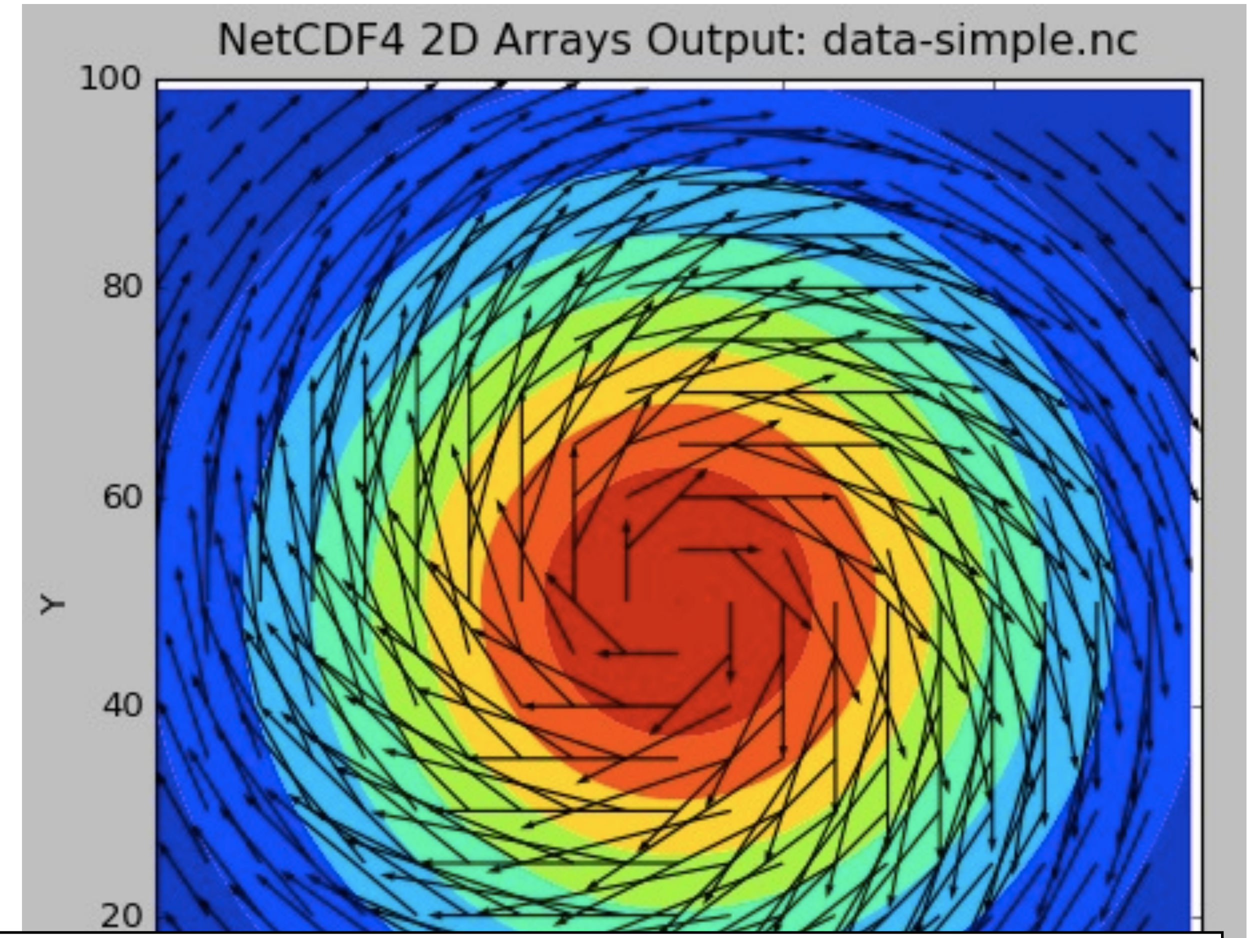



```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ components = 2 ;
variables:
  double Density(Y, X) ;
  double Velocity(Y, X, velocity\
```

NetCDF

- NetCDF is a set of libraries and formats for:
  - portable,
  - efficient
  - “self-describing”
- way of storing and accessing large arrays (eg, for scientific data)

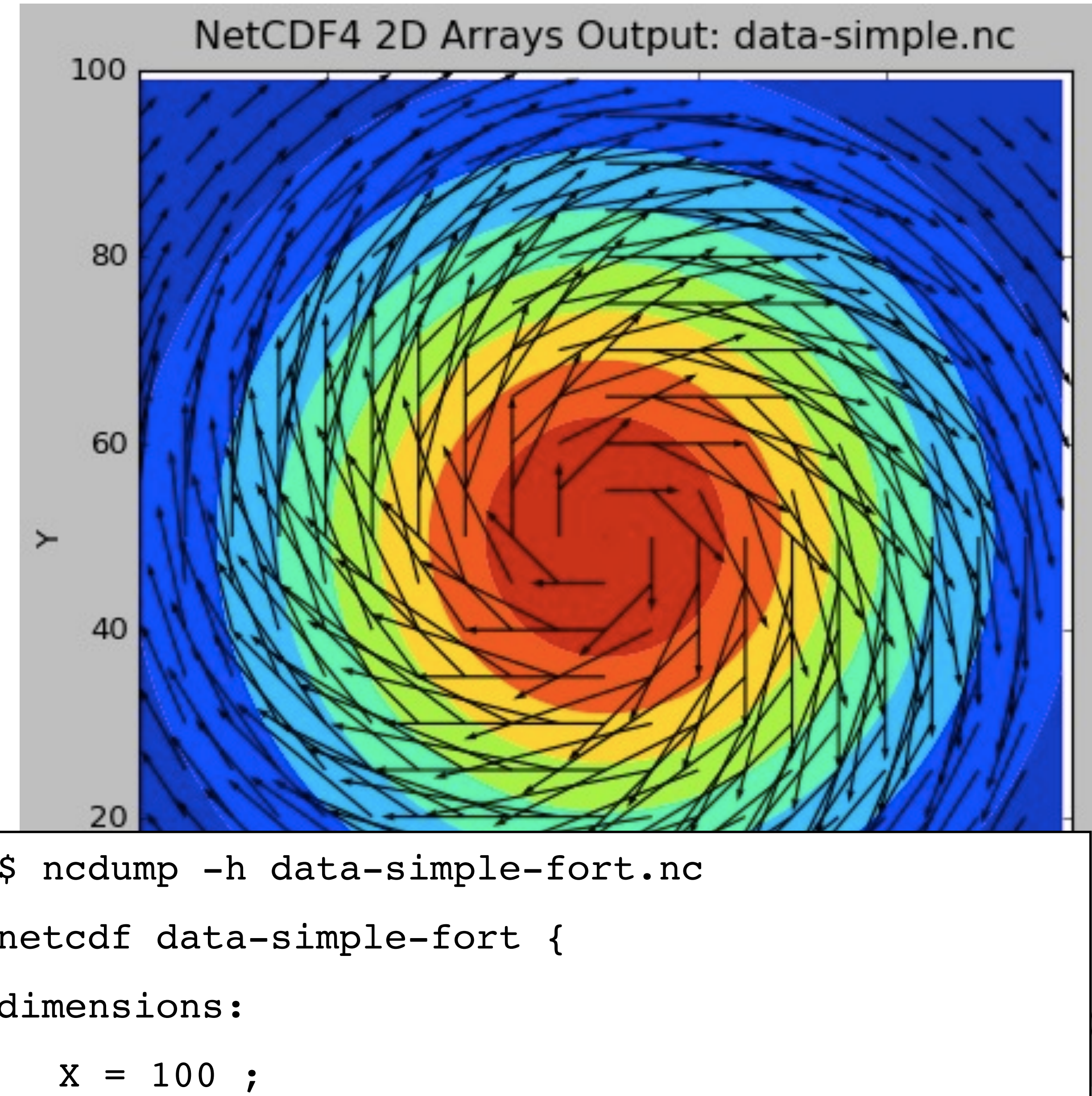
- Current version is NetCDF4




```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity\ components = 2 ;
variables:
   double Density(Y, X) ;
   double Velocity(Y, X, velocity\
components) ;
}
```

NetCDF: *Portable*

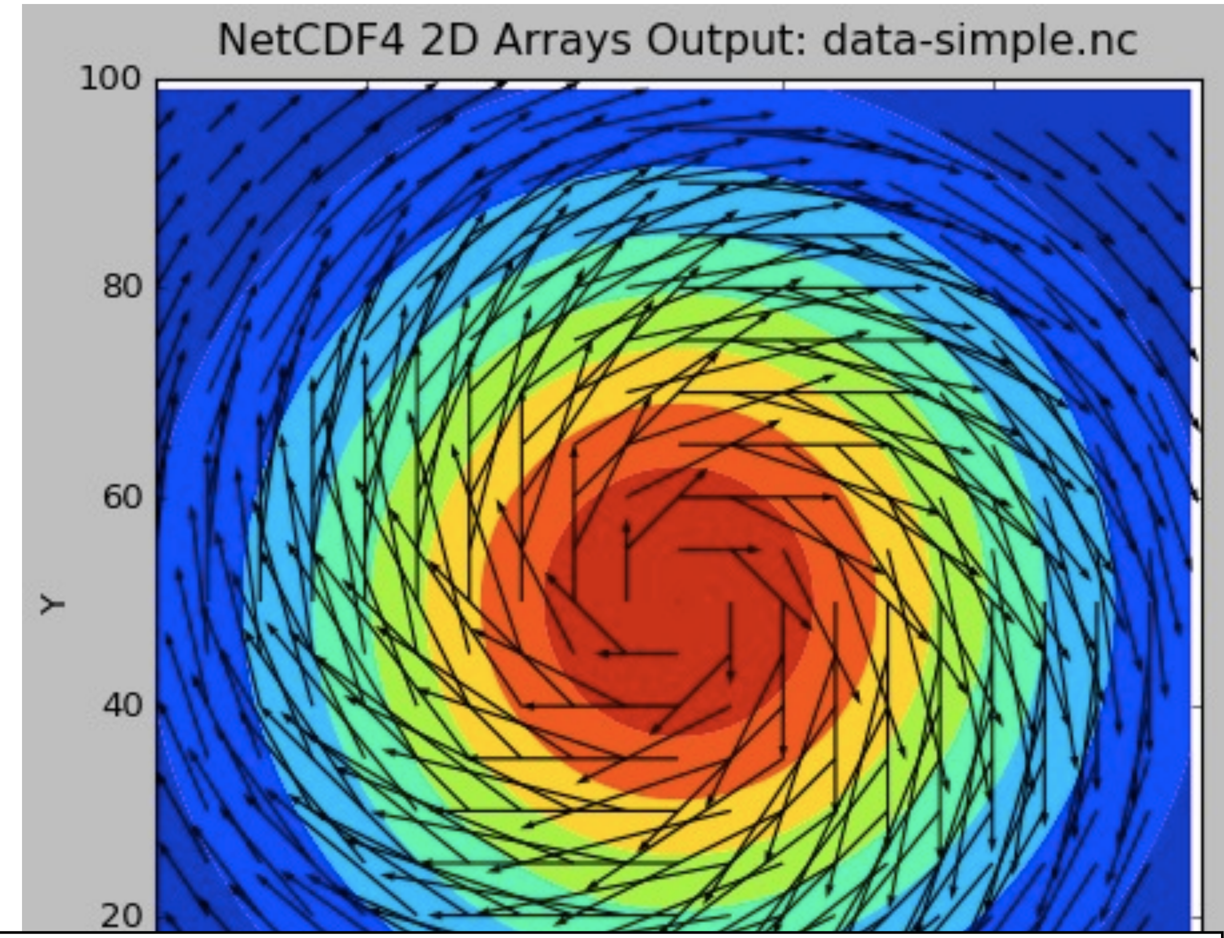
- Binary files, but common output format so that different sorts of machines can share files.
- Libraries accessible from C, C++, Fortran-77, Fortran 90/95/2003, python, etc.




```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity\ components = 2 ;
variables:
   double Density(Y, X) ;
   double Velocity(Y, X, velocity\
components) ;
}
```

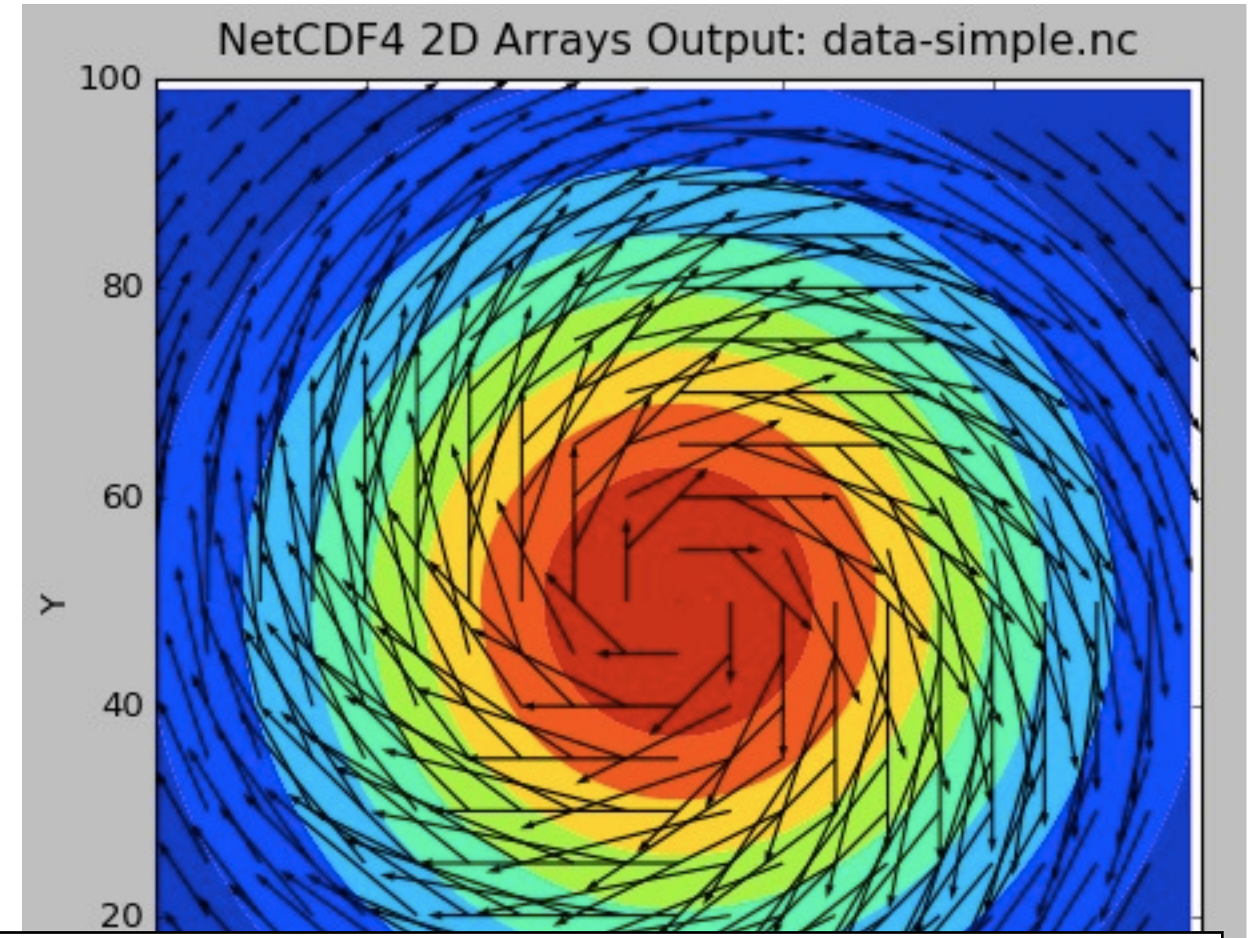
NetCDF: *Self-Describing*

- Header contains the metadata to describe the big data
- Lists:
  - Array names
  - Dimensions
  - *shared* dimensions - information about how the arrays relate
  - Other, related information




```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity\ components = 2 ;
variables:
   double Density(Y, X) ;
   double Velocity(Y, X, velocity\
components) ;
}
```

NetCDF: *Efficient*



- Binary, so less translation (as little is used as possible)
- IO libraries themselves are written for performance
- API, data format makes it easy to efficiently read,write subregions of arrays (slices, or 'hyperslabs')
- Still possible to make things slow - lots of metadata queries, modifications

```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity\ components = 2 ;
variables:
   double Density(Y, X) ;
   double Velocity(Y, X, velocity\
components) ;
}
```

2darray-simple.c

```
#include "netcdf.h"

...

void writenetcdffile(rundata_t rundata, double **dens,
                     double ***vel) {
    /* identifiers */
    int file_id;

...
    /* return status */
    int status;

    /* Create a new file - clobber anything existing */
    status = nc_create(rundata.filename, NC_CLOBBER, &file_id);
    /* netCDF routines return NC_NOERR on success */
    if (status != NC_NOERR) {
        fprintf(stderr,"Could not open file %s\n", rundata.filename);
```

Include function definitions

2darray-simple.c

```
#include "netcdf.h"

...

void writenetcdffile(rundata_t rundata, double **dens,
                     double ***vel) {
    /* identifiers */
    int file_id;

...
    /* return status */
    int status;

    /* Create a new file - clobber anything existing */
    status = nc_create(rundata.filename, NC_CLOBBER, &file_id);
    /* netCDF routines return NC_NOERR on success */
    if (status != NC_NOERR) {
        fprintf(stderr,"Could not open file %s\n", rundata.filename);
```

Create a new file, with name rundata.filename

2darray-simple.c

```
#include "netcdf.h"

...

void writenetcdffile(rundata_t rundata, double **dens,
                     double ***vel) {
    /* identifiers */
    int file_id;

...
    /* return status */
    int status;

    /* Create a new file - clobber anything existing */
    status = nc_create(rundata.filename, NC_CLOBBER, &file_id);
    /* netCDF routines return NC_NOERR on success */
    if (status != NC_NOERR) {
        fprintf(stderr,"Could not open file %s\n", rundata.filename);
```

Clobber anything already in the file

2darray-simple.c

```
#include "netcdf.h"

...

void writenetcdffile(rundata_t rundata, double **dens,
                     double ***vel) {
    /* identifiers */
    int file_id;

...
    /* return status */
    int status;

    /* Create a new file - clobber anything existing */
    status = nc_create(rundata.filename, NC_CLOBBER, &file_id);
    /* netCDF routines return NC_NOERR on success */
    if (status != NC_NOERR) {
        fprintf(stderr,"Could not open file %s\n", rundata.filename);
```

Test the return codes

f2darray-simple.f90

```
subroutine writenetcdffile(rundata, dens, vel)
     use netcdf
     implicit none
     type(rundata_t), intent(IN) :: rundata
     double precision, intent(IN), dimension(:,:) :: dens
     double precision, intent(IN), dimension(:,:,:) :: vel

     integer :: file_id
...
     integer :: status

     ! create the file, check return code

     status = nf90_create(path=rundata%filename, cmode=NF90_CLOBBER,
ncid=file_id)
     if (status /= NF90_NOERR) then
         print *,'Could not open file ', rundata%filename
     return
```

Import definitions

f2darray-simple.f90

```
subroutine writenetcdffile(rundata, dens, vel)
     use netcdf
     implicit none
     type(rundata_t), intent(IN) :: rundata
     double precision, intent(IN), dimension(:,:) :: dens
     double precision, intent(IN), dimension(:,:,:) :: vel

     integer :: file_id
...
     integer :: status

     ! create the file, check return code

     status = nf90_create(path=rundata%filename, cmode=NF90_CLOBBER,
ncid=file_id)
     if (status /= NF90_NOERR) then
         print *,'Could not open file ', rundata%filename
     return
```

Create file

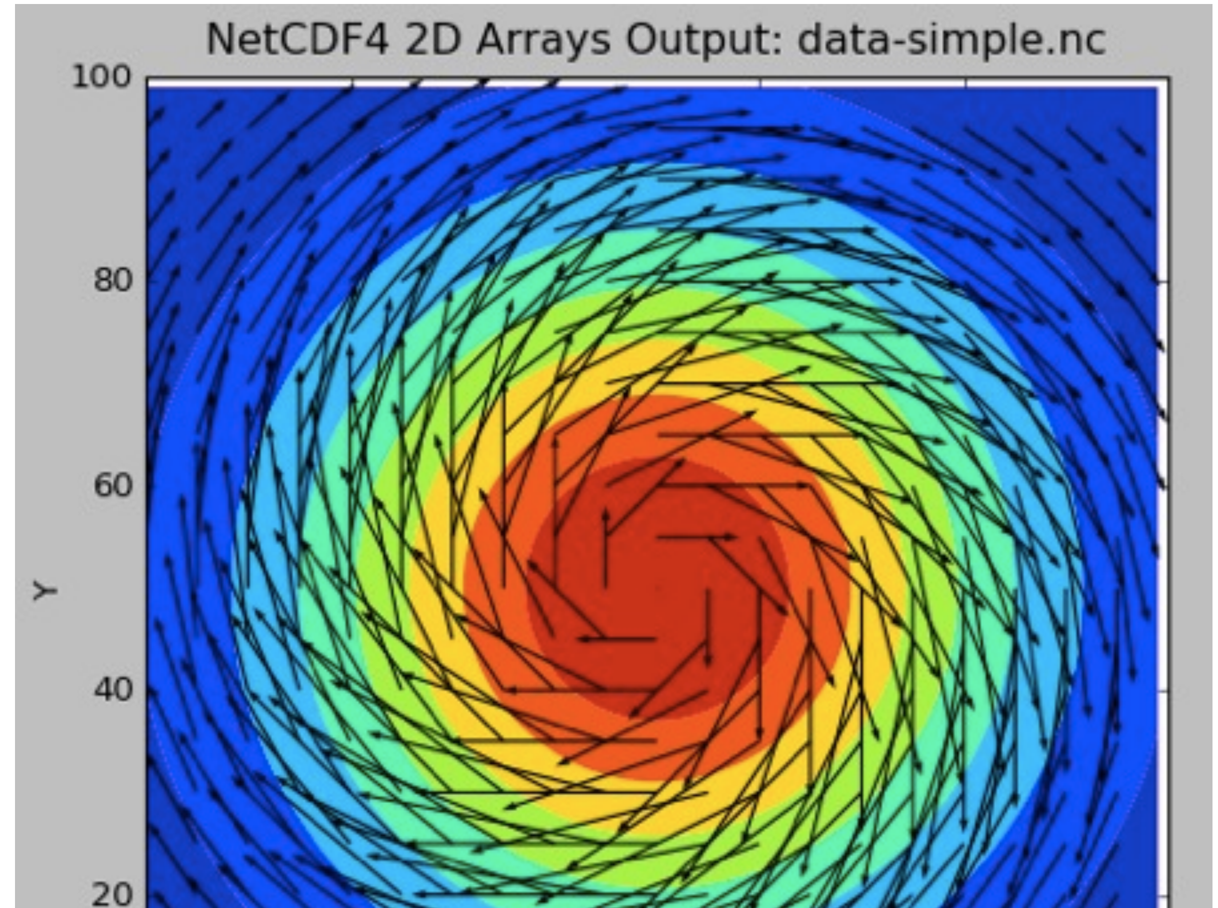
f2darray-simple.f90

```
subroutine writenetcdffile(rundata, dens, vel)
     use netcdf
     implicit none
     type(rundata_t), intent(IN) :: rundata
     double precision, intent(IN), dimension(:,:) :: dens
     double precision, intent(IN), dimension(:,:,:) :: vel

     integer :: file_id
...
     integer :: status

     ! create the file, check return code

     status = nf90_create(path=rundata%filename, cmode=NF90_CLOBBER,
ncid=file_id)
     if (status /= NF90_NOERR) then
         print *,'Could not open file ', rundata%filename
     return
```

C definitions are NC_, F90 are NF90_

Writing a NetCDF File

- To write a NetCDF file, we go through the following steps:
  - **Create** the file (or open it for appending)
  - **Define dimensions** of the arrays we'll be writing
  - **Define variables** on those dimensions
  - **End definition** phase
  - **Write variables**
  - **Close file**




```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
    X = 100 ;
    Y = 100 ;
    velocity\ components = 2 ;
variables:
    double Density(Y, X) ;
    double Velocity(Y, X, velocity\ components) ;
}
```

f2darray-simple.f90

```
integer :: file_id, xdim_id, ydim_id, vcomp_id
integer :: dens_id, vel_id
integer, dimension(2) :: densdims
integer, dimension(3) :: veldims

...

status = nf90_def_dim(file_id, 'X', rundata%nx, xdim_id)
status = nf90_def_dim(file_id, 'Y', rundata%ny, ydim_id)
status = nf90_def_dim(file_id, 'velocity components', 2, vcomp_id)

densdims = (/ xdim_id, ydim_id /)
veldims = (/ vcomp_id, xdim_id, ydim_id /)

status = nf90_def_var(file_id, 'Density',  NF90_DOUBLE, densdims, dens_id)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Dens'
status = nf90_def_var(file_id, 'Velocity', NF90_DOUBLE, veldims,  vel_id)

status = nf90_enddef(file_id)
```

Define the dimensions in the file: name, size, id

f2darray-simple.f90

```
integer :: file_id, xdim_id, ydim_id, vcomp_id
integer :: dens_id, vel_id
integer, dimension(2) :: densdims
integer, dimension(3) :: veldims

...

status = nf90_def_dim(file_id, 'X', rundata%nx, xdim_id)
status = nf90_def_dim(file_id, 'Y', rundata%ny, ydim_id)
status = nf90_def_dim(file_id, 'velocity components', 2, vcomp_id)

densdims = (/ xdim_id, ydim_id /)
veldims = (/ vcomp_id, xdim_id, ydim_id /)

status = nf90_def_var(file_id, 'Density',  NF90_DOUBLE, densdims, dens_id)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Dens'
status = nf90_def_var(file_id, 'Velocity', NF90_DOUBLE, veldims,  vel_id)

status = nf90_enddef(file_id)
```

Variables are defined in terms of these dims

f2darray-simple.f90

Once you're done defining things,

```
status = nf90_enddef(file_id)

! Write out the values
status = nf90_put_var(file_id, dens_id, dens)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Dens'
status = nf90_put_var(file_id, vel_id,  vel)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Vel'

status = nf90_close(file_id)
```

f2darray-simple.f90

Writing data is easy.

```
status = nf90_enddef(file_id)

! Write out the values
status = nf90_put_var(file_id, dens_id, dens)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Dens'
status = nf90_put_var(file_id, vel_id,  vel)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Vel'

status = nf90_close(file_id)
```

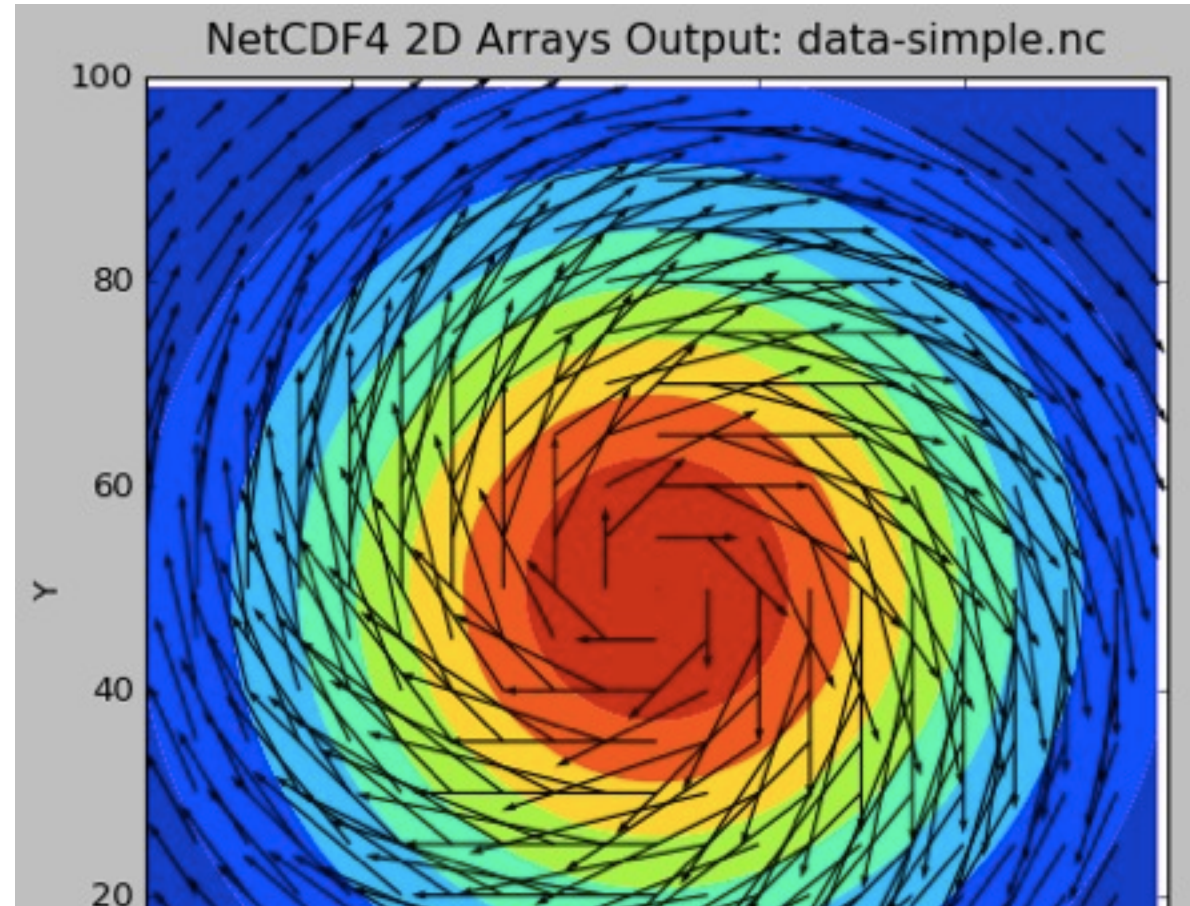
f2darray-simple.f90

```
status = nf90_enddef(file_id)

! Write out the values
status = nf90_put_var(file_id, dens_id, dens)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Dens'
status = nf90_put_var(file_id, vel_id,  vel)
if (status /= NF90_NOERR) print *, trim(nf90_strerror(status)), ' Vel'

status = nf90_close(file_id)
```

Closing the file is important!!

Reading a NetCDF File

- Flow is slightly different
  - **Open** the file for reading
  - **Get dimension ids** of the the dimensions in the files
  - **Get dimension lengths** so you can allocate the files
  - **Get variable ids** so you can access the data
  - **Read variables**
  - **Close file**




```
$ ncdump -h data-simple-fort.nc
netcdf data-simple-fort {
dimensions:
    X = 100 ;
    Y = 100 ;
    velocity\ components = 2 ;
variables:
    double Density(Y, X) ;
    double Velocity(Y, X, velocity\ components) ;
}
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

fread2darray-simple.f90

```
status = nf90_open(path=rundata%filename, mode=NF90_NOWRITE, ncid=file_id)
...
! find the dimensions
status = nf90_inq_dimid(file_id, 'X', xdim_id)
status = nf90_inq_dimid(file_id, 'Y', ydim_id)
status = nf90_inq_dimid(file_id, 'velocity components', vcomp_id)
! find the dimension lengths
status = nf90_inquire_dimension(file_id, xdim_id, len = rundata % nx)
status = nf90_inquire_dimension(file_id, ydim_id, len = rundata % ny )
status = nf90_inquire_dimension(file_id, vcomp_id,len = rundata % nvelcomp)
! now we can allocate variable sizes
allocate(dens(rundata%nx, rundata%ny)) !...etc...

status = nf90_inq_varid(file_id, 'Density',  dens_id)
status = nf90_inq_varid(file_id, 'Velocity', vel_id)

status = nf90_get_var(file_id, dens_id, dens)
status = nf90_get_var(file_id, vel_id,  vel)

status = nf90_close(file_id)
```

read2darray-simple.c

```
status = nc_open(rundata->filename, NC_NOWRITE, &file_id);

/* Get the dimensions */
status = nc_inq_dimid(file_id, "X", &xdim_id);
if (status != NC_NOERR) fprintf(stderr, "Could not get X\n");
status = nc_inq_dimid(file_id, "Y", &ydim_id);
status = nc_inq_dimid(file_id, "velocity component", &vcomp_id);

status = nc_inq_dimlen(file_id, xdim_id, &(rundata->nx));
status = nc_inq_dimlen(file_id, ydim_id, &(rundata->ny));
status = nc_inq_dimlen(file_id, vcomp_id, &(rundata->nveldims));

...
nc_inq_varid(file_id, "Density", &dens_id);
nc_inq_varid(file_id, "Velocity", &vel_id);

nc_get_var_double(file_id, dens_id, &((*dens)[0][0]));
nc_get_var_double(file_id, vel_id, &((*vel)[0][0][0]));

nc_close(file_id);
```

A Better example

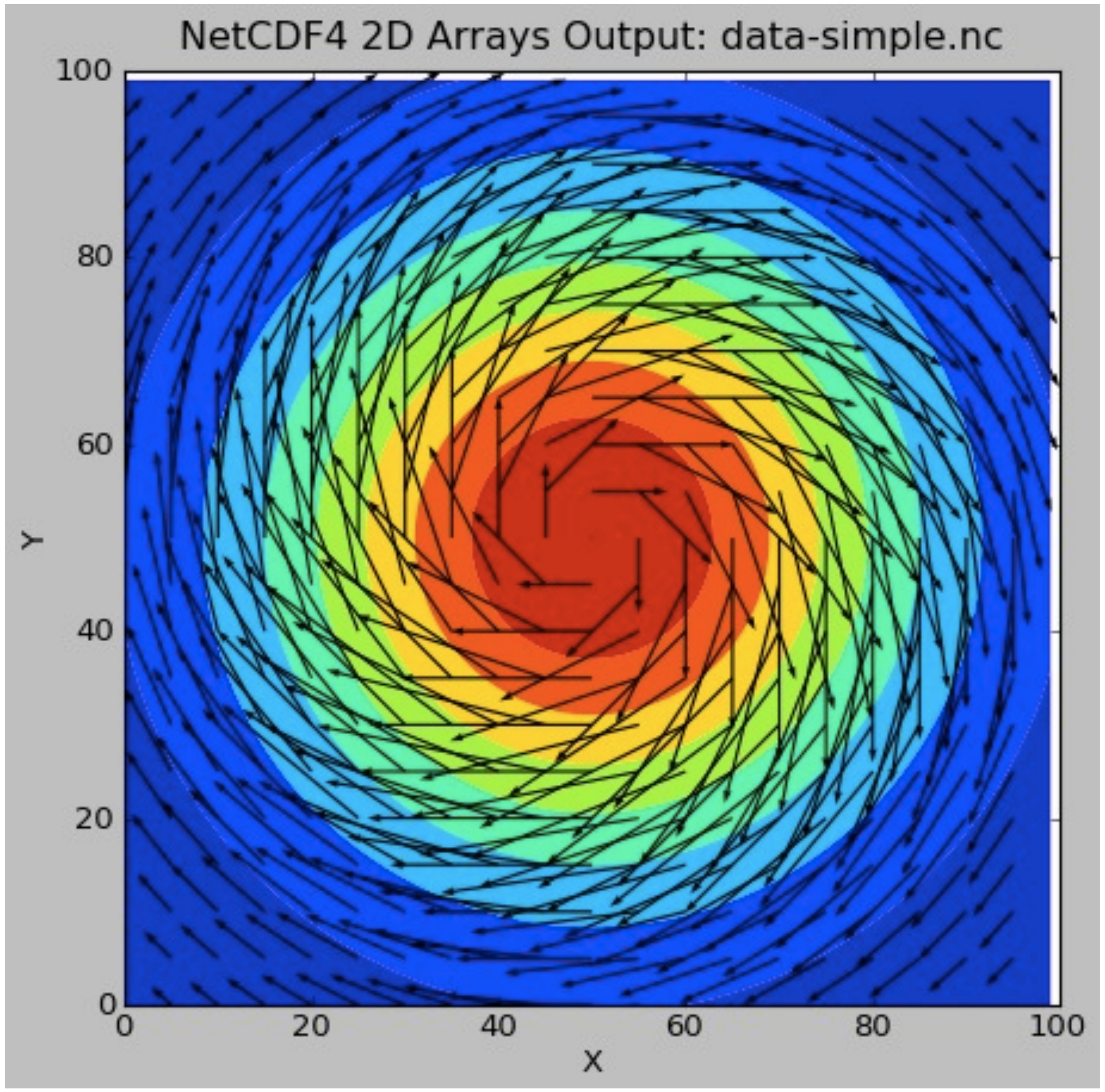
- The above example is much more austere than a typical NetCDF file
- A more typical example is given in 2darray (or f2darray)
- make this, then run it
- ../plots.py data.nc
- (Same options as previous example)

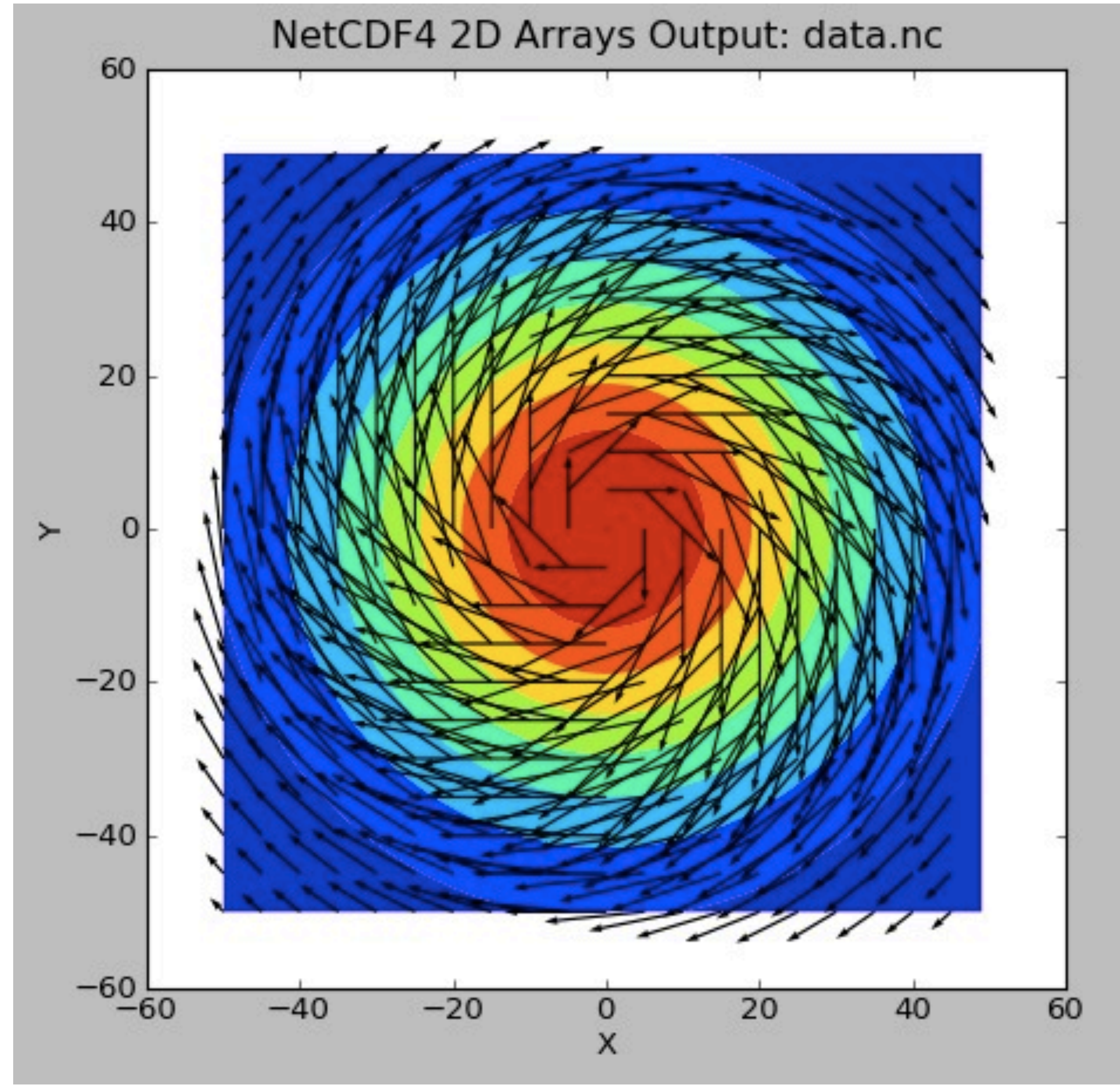
```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
     X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
     Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
     Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
     Velocity:units = "cm/s" ;
}
```

2darray.c

```
float *x, *y;
const char *coordunit="cm";
...
for (i=0; i<rundata.nx; i++) x[i] = (1.*i-r
for (i=0; i<rundata.ny; i++) y[i] = (1.*i-r
...
/* define the dimensions */
nc_def_dim(file_id, "X", rundata.nx, &xdim_id);
nc_def_dim(file_id, "Y", rundata.ny, &ydim_id);
nc_def_dim(file_id, "velocity component", 2, &vcomp_id);

/* define the coordinate variables,... */
nc_def_var(file_id, "X coordinate", NC_FLOAT, 1, &xdim_id, &xcoord_id);
nc_def_var(file_id, "Y coordinate", NC_FLOAT, 1, &ydim_id, &ycoord_id);

/* ...and assign units to them as an attribute */
nc_put_att_text(file_id, xcoord_id, "units", strlen(coordunit), coordunit);
nc_put_att_text(file_id, ycoord_id, "units", strlen(coordunit), coordunit);
```

Typically not only define dimensions but give coordinate values


NetCDF4 2D Arrays Output: data-simple.nc
Y
X
0
20
40
60
80
100


NetCDF4 2D Arrays Output: data.nc
Y
X
−60
−40
−20
0
20
40
60

2darray.c

Variables (or anything else) can have **attributes:** Name, and arbitrary data

```
float *x, *y;
const char *coordunit="cm";
...
for (i=0; i<rundata.nx; i++) x[i] = (1.*i-r
for (i=0; i<rundata.ny; i++) y[i] = (1.*i-r
...
/* define the dimensions */
nc_def_dim(file_id, "X", rundata.nx, &xdim_id);
nc_def_dim(file_id, "Y", rundata.ny, &ydim_id);
nc_def_dim(file_id, "velocity component", 2, &vcomp_id);

/* define the coordinate variables,... */
nc_def_var(file_id, "X coordinate", NC_FLOAT, 1, &xdim_id, &xcoord_id);
nc_def_var(file_id, "Y coordinate", NC_FLOAT, 1, &ydim_id, &ycoord_id);

/* ...and assign units to them as an attribute */
nc_put_att_text(file_id, xcoord_id, "units", strlen(coordunit), coordunit);
nc_put_att_text(file_id, ycoord_id, "units", strlen(coordunit), coordunit);
```

NetCDF Attributes

- Any NetCDF object (data set, dimension) can have an arbitrary number of attributes associated with it
- Name, and any type or size...
- Like a variable! (But can't access only part of it).

```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
     X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
     Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
     Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
     Velocity:units = "cm/s" ;
}
```

NetCDF Attributes

- Attributes are assumed to be “small”, though.
- Stored in header information (not with big data)
- Don’t put large arrays in there

```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
     X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
     Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
     Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
     Velocity:units = "cm/s" ;
}
```

NetCDF Attributes

- Units are particularly useful attributes, as if a code needs data in some other units (MKS), can convert.

```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
     X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
     Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
     Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
     Velocity:units = "cm/s" ;
}
```

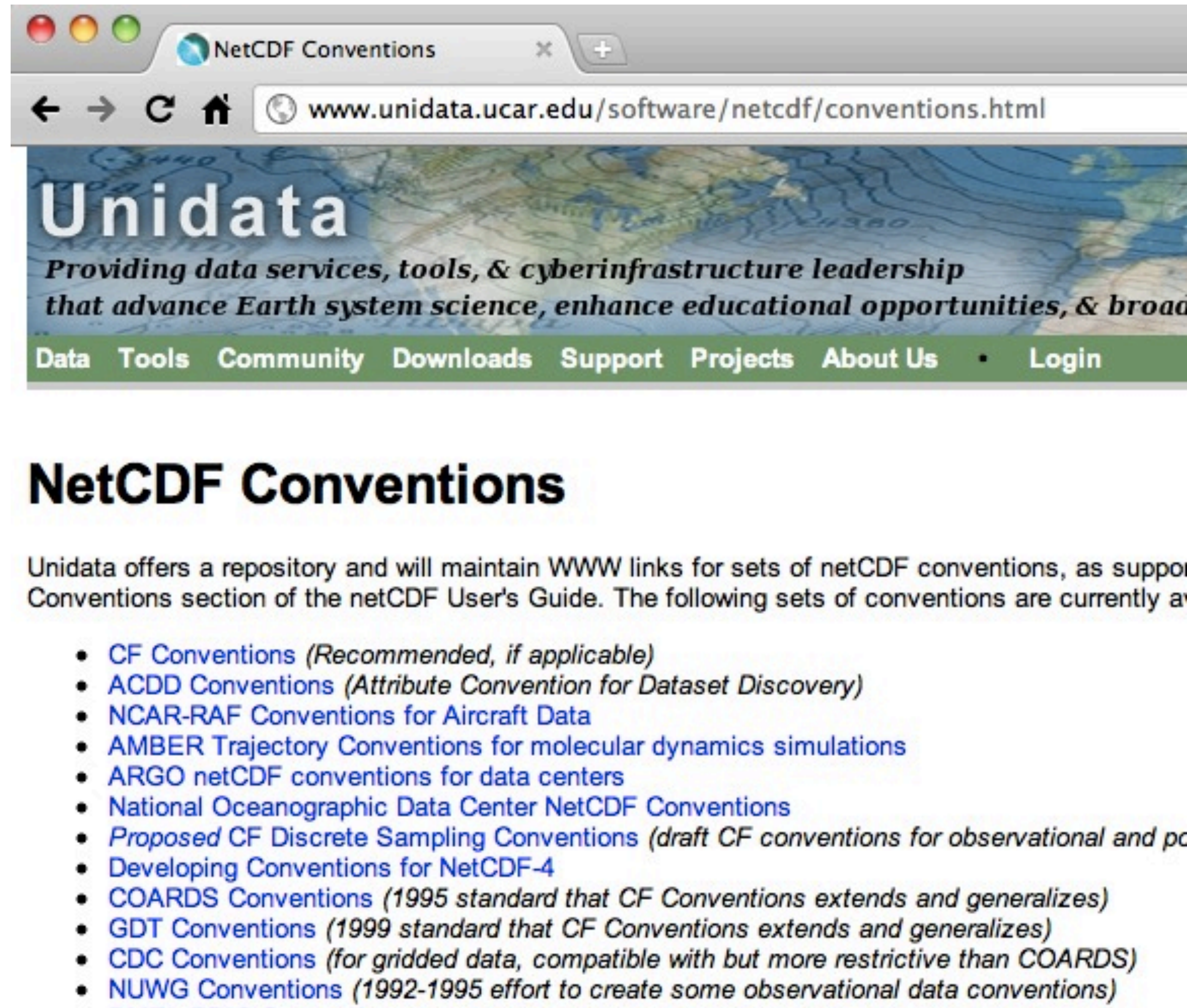
Limits to Self-Description

- But what if some codes expect "centimetre" and you use cm?
- Or their code uses "Dens" or "Rho" and yours uses "Density?" Or uses momentum rather than velocity?

```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
     X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
     Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
     Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
     Velocity:units = "cm/s" ;
}
```

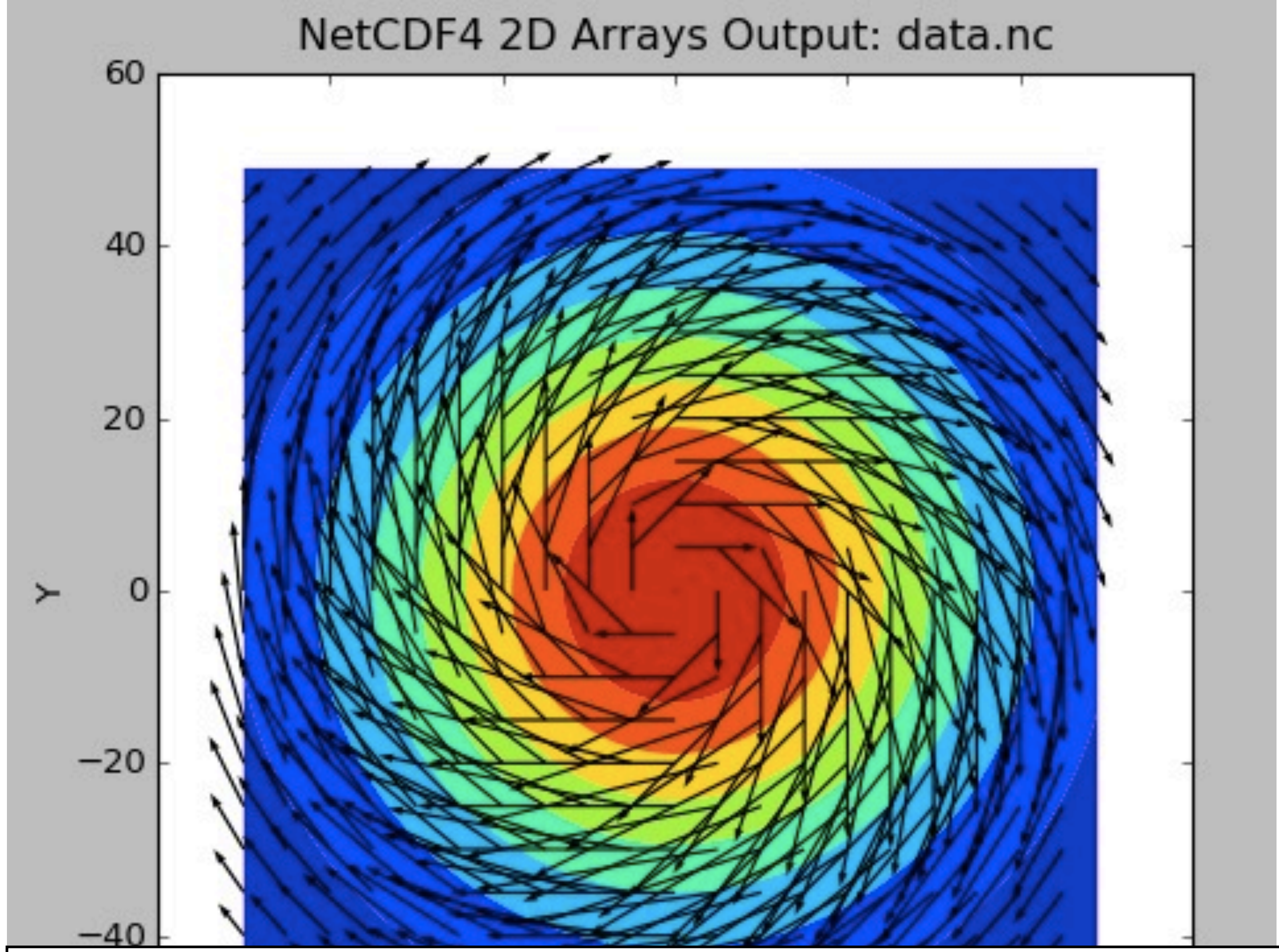
Conventions

- There are lists of conventions that you can follow for variable names, unit names, etc.
- If you are planning for interoperability with other codes, this is the way to go
- Codes expecting data following (say) CF conventions for geophys should recognize data in that convention



Big advantage of self-describing:

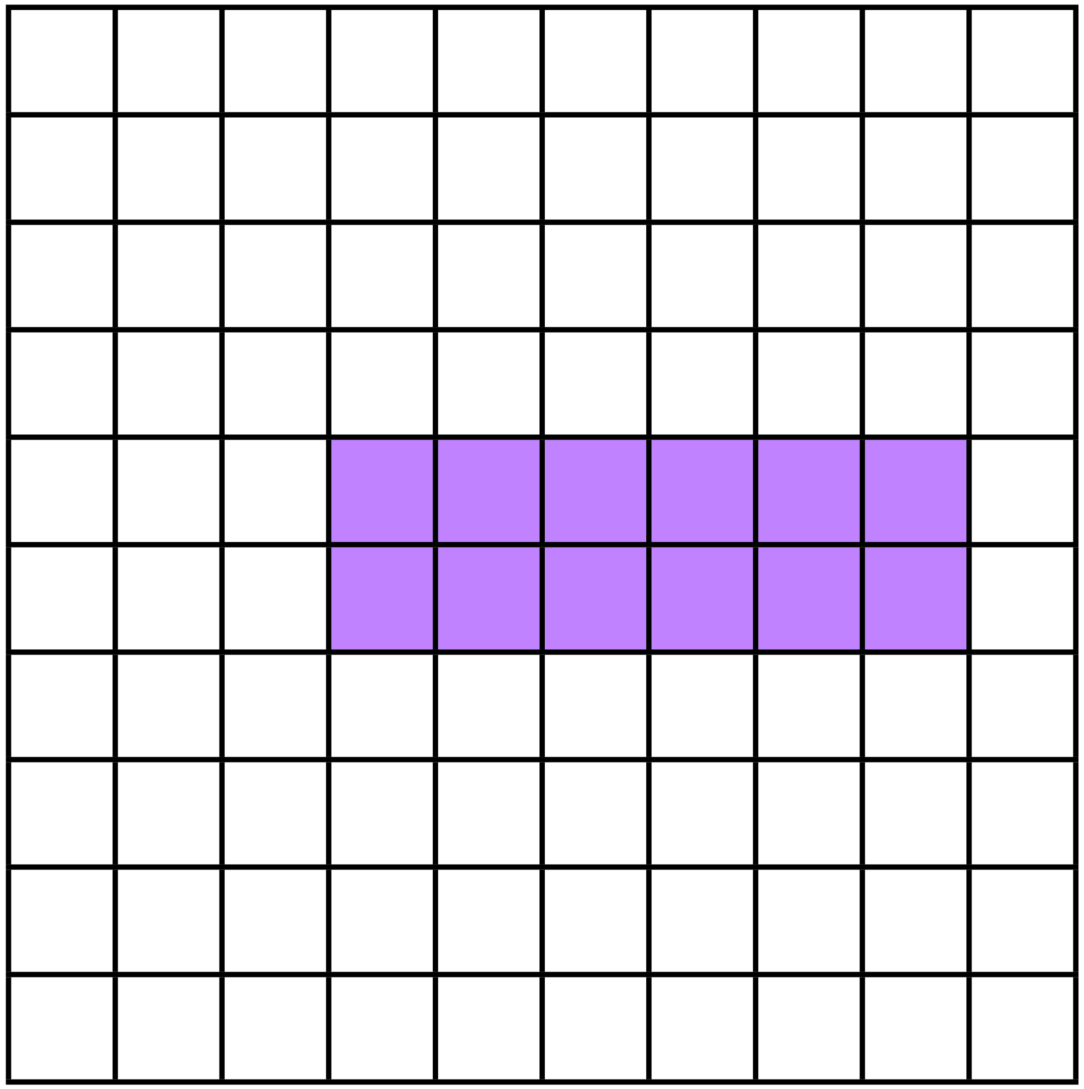
- Old program could easily read new file, even though data layout changed!
- Doesn't even need to know about attributes...
- New variables don't cause any problems - don't have to read them!
- Backwards compatibility
- But can look for them and use if available.



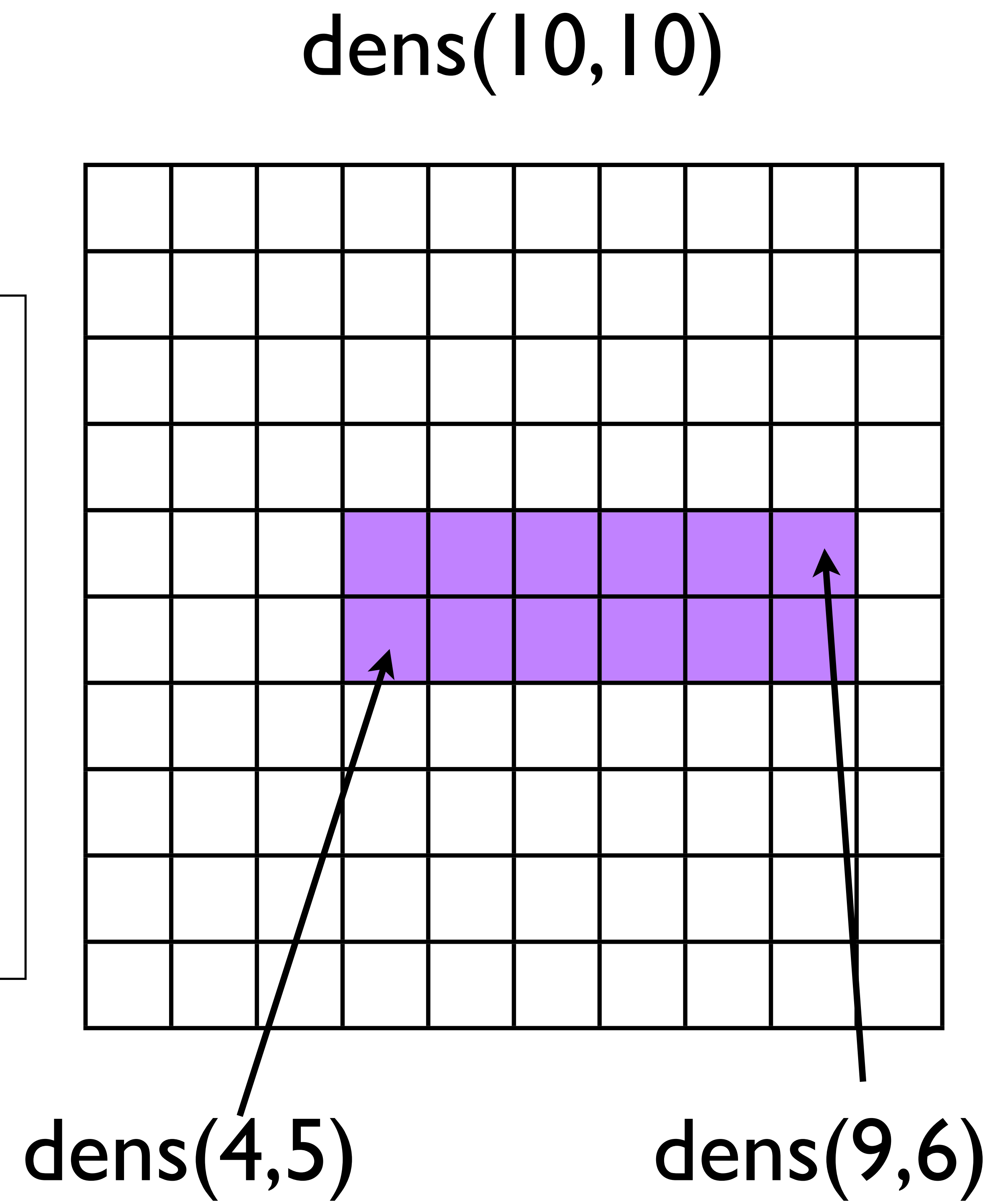

```
$ ncdump -h data.nc
netcdf data {
dimensions:
   X = 100 ;
   Y = 100 ;
   velocity\ component = 2 ;
variables:
   float X\ coordinate(X) ;
        X\ coordinate:units = "cm" ;
   float Y\ coordinate(Y) ;
        Y\ coordinate:units = "cm" ;
   double Density(X, Y) ;
        Density:units = "g/cm^3" ;
   double Velocity(velocity\ component, X, Y
        Velocity:units = "cm/s" ;
}
```

Accessing subregions in file

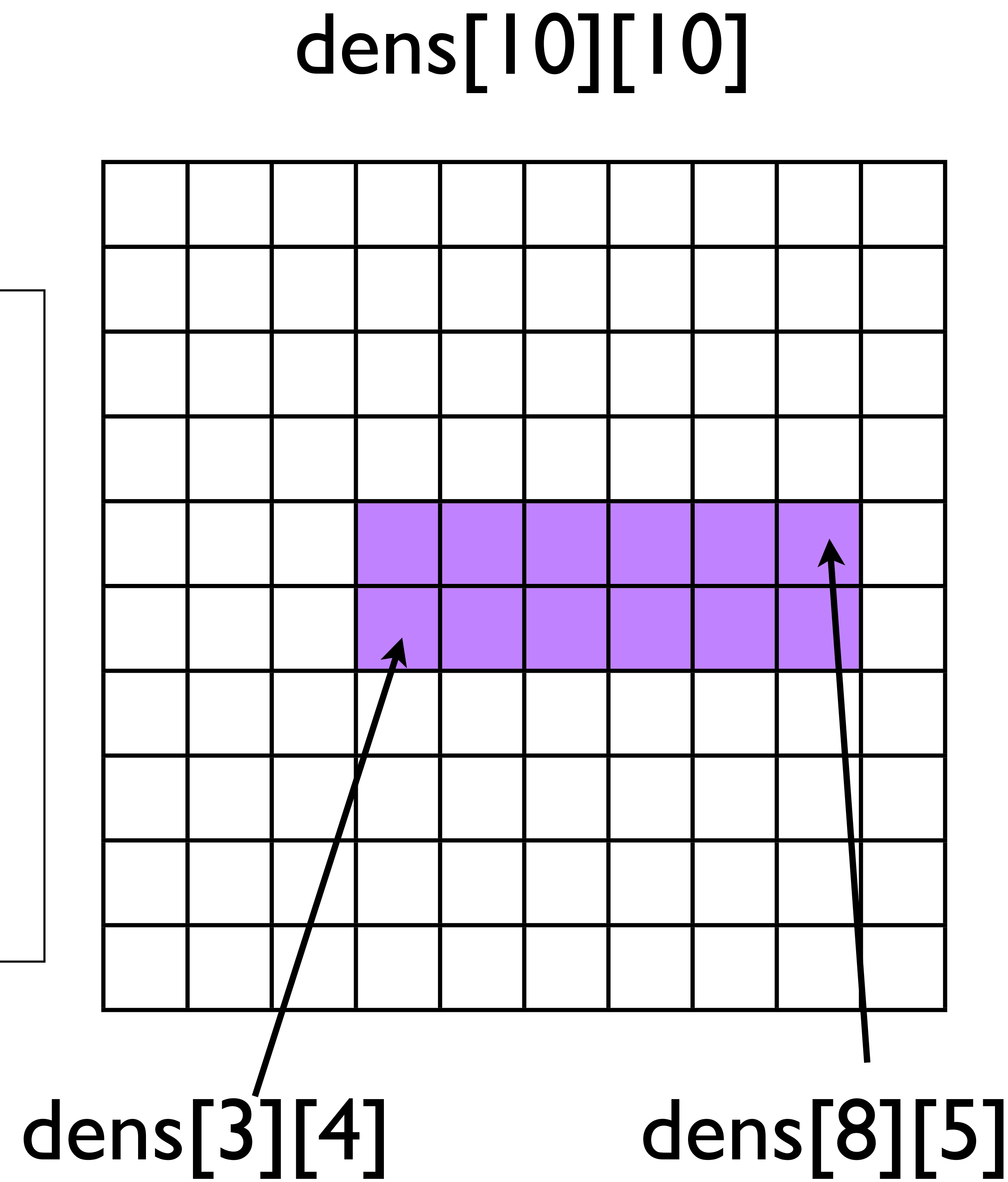
- nc_put_var_type or nf90_put_var puts whole array(by default)
- Subarrays can be specified with starts and counts



```
start(1) = 4
start(2) = 5

count(1) = 6
count(2) = 2

nf90_put_var(file_id, dens_id,
data, START=start, COUNT=count)
```

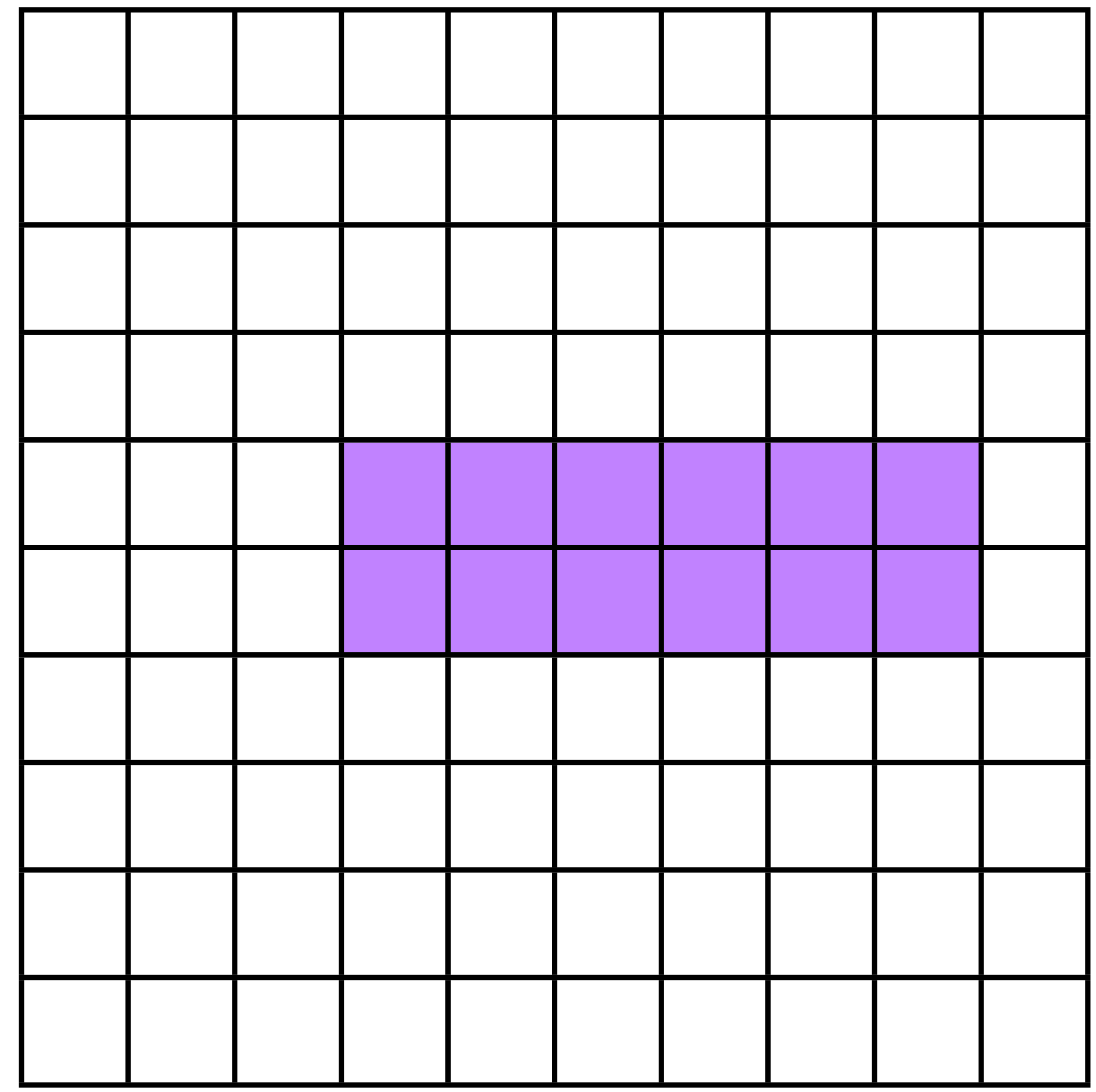


```
start[0] = 3;
start[1] = 4;

count[0] = 6;
count[1] = 2;

nc_put_vara_double(file_id,
dens_id, start, count, data);
```



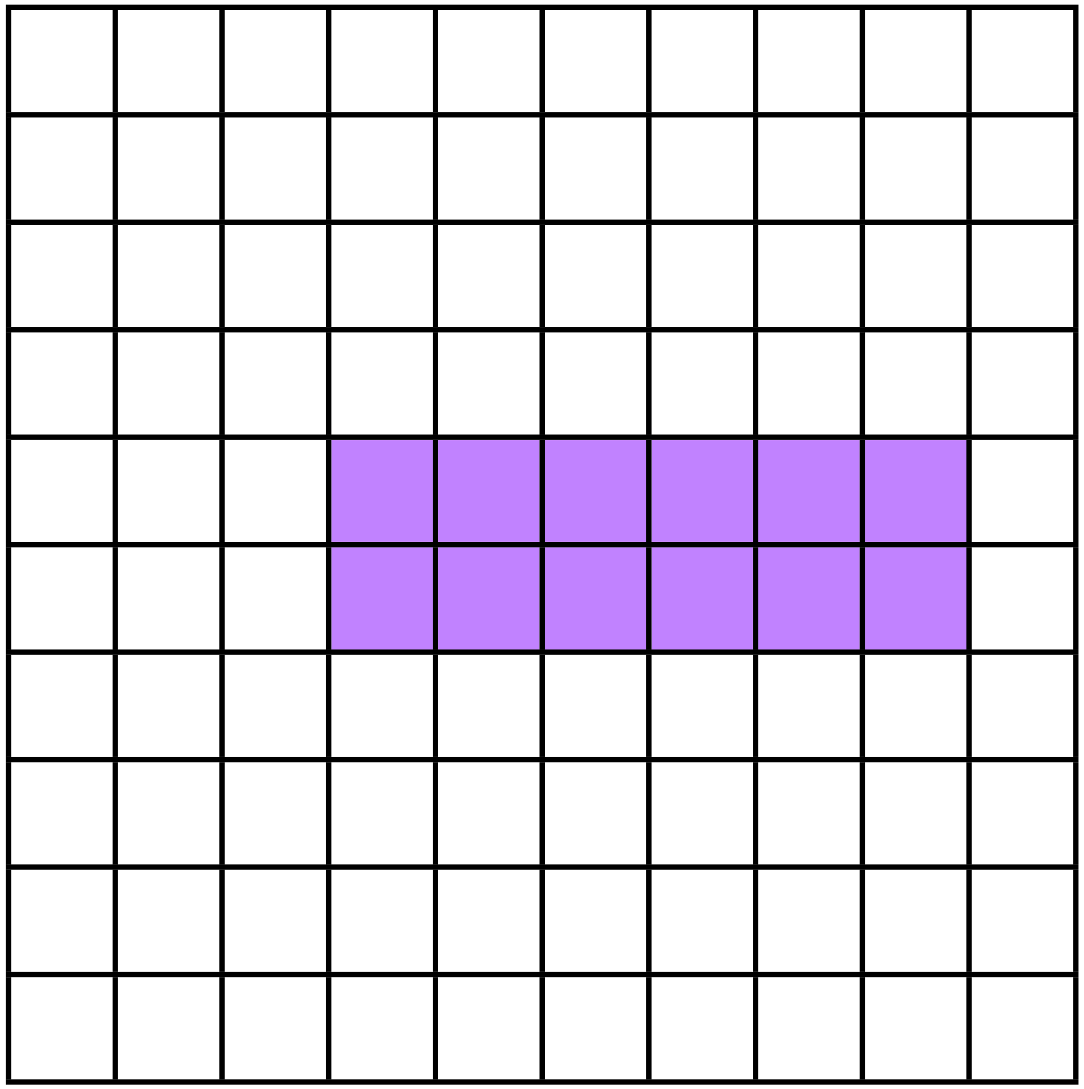
Accessing subregions in file

- Note that NetCDF libraries accepts starting conventions of C, Fortran as appropriate.



Accessing subregions in file

- Another thing this is good for; arrays in NetCDF can have a dimension of unlimited size (eg, can grow) - NetCDF3, only one dimension, NetCDF4, any
- Can use for timesteps, for instance.
- Any access to such a dataset is necessarily via subregions.



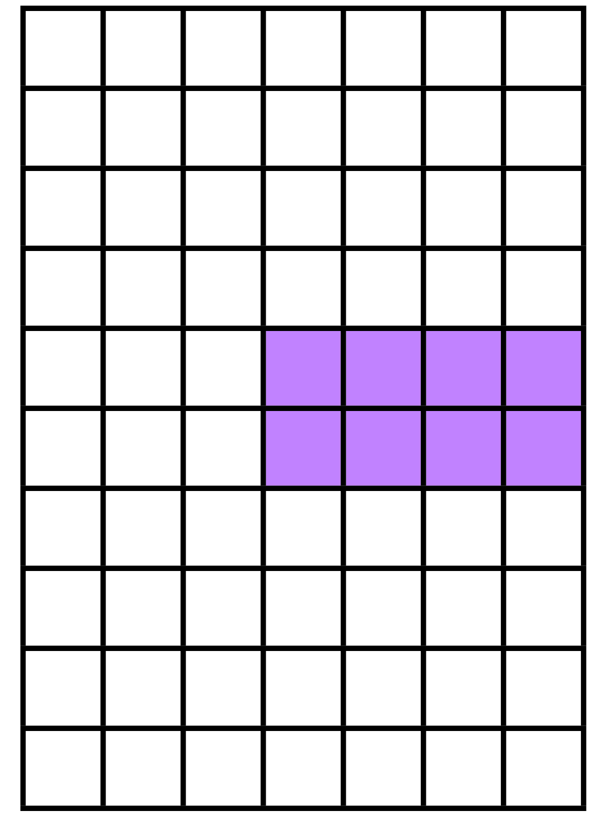
Fortran vs C array conventions

```
$ ncdump -h data.nc
netcdf data {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ component = 2 ;
variables:
  float X\ coordinate(X) ;
      X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
      Y\ coordinate:units = "cm" ;
  double Density(X, Y) ;
      Density:units = "g/cm^3" ;
  double Velocity(velocity\
component, X, Y) ;
      Velocity:units = "cm/s" ;
}
```

```
$ ncdump -h data-fort.nc
netcdf data-fort {
dimensions:
  X = 100 ;
  Y = 100 ;
  velocity\ components = 2 ;
variables:
  float X\ coordinate(X) ;
      X\ coordinate:units = "cm" ;
  float Y\ coordinate(Y) ;
      Y\ coordinate:units = "cm" ;
  double Density(Y, X) ;
      Density:units = "g/cm^3" ;
  double Velocity(Y, X, velocity\
components) ;
      Velocity:units = "cm/s" ;
}
```

Mapping memory space to file

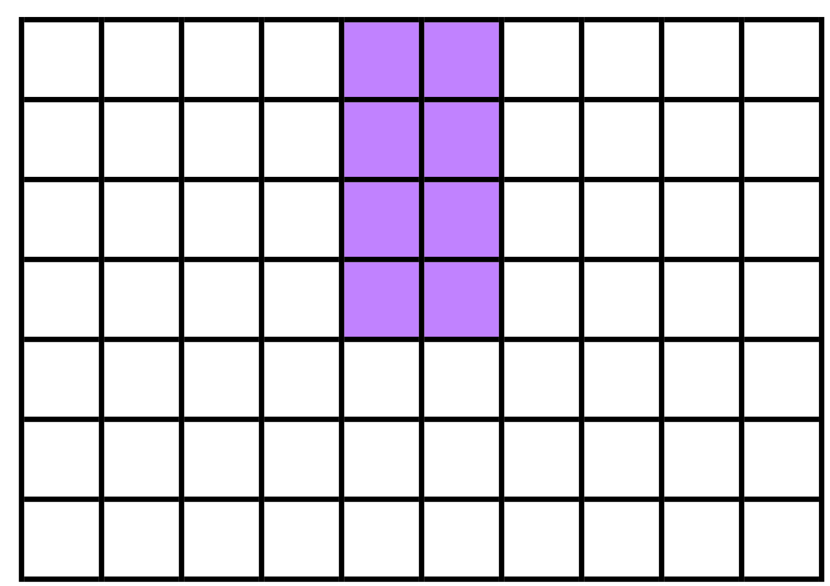
- Say in C you wanted to output in FORTRAN convention
- (i,j) in your array corresponds to (j,i) in data space in file
- nc_put_var**m** allows you to do this by mapping how indicies vary in memory compared to in file.



dens[7][10]

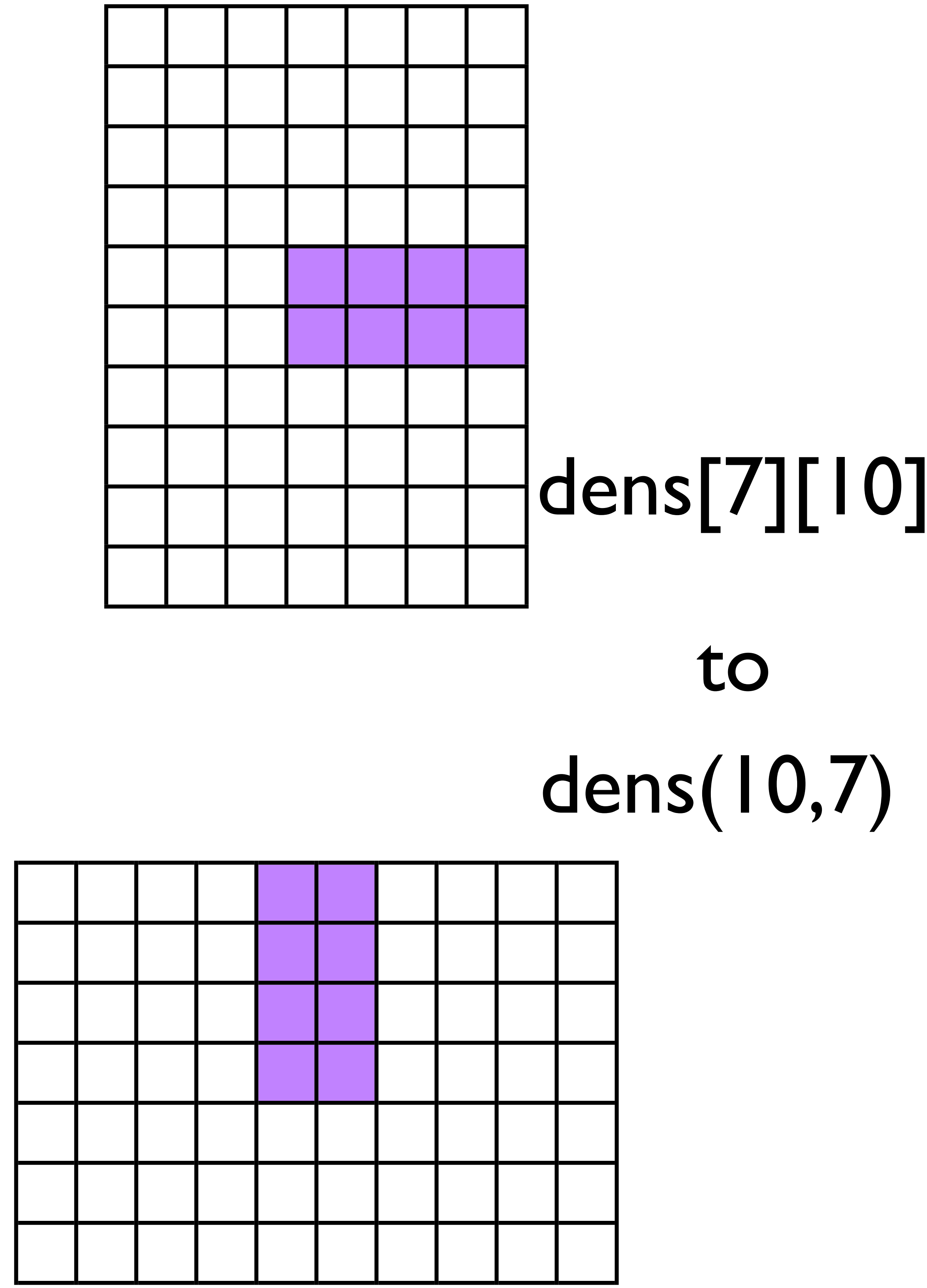
to

dens(10,7)



Mapping memory space to file

- Note - this requires understanding how memory is laid out in your data structures, as with MPI & MPI-IO
- This is *crucial* for I/O, and for HPC in general
- C has more flexibility (== potential problems) in this regard.



Mapping memory space to file

- C: first array index most slowly varying.
- Eg, for a 3x4 array, each step in the 2nd index jumps you one position in memory,
- and in the first index, jumps you by 4.
- You could write this as (4,1)

Your picture of the array

[2][0]	[2][1]	[2][2]	[2][3]
[1][0]	[1][1]	[1][2]	[1][3]
[0][0]	[0][1]	[0][2]	[0][3]

In memory

[0][0]	[0][1]	[0][2]	[0][3]	[1][0]	[1][1]	[1][2]	[1][3]	[2][0

Mapping memory space to file

- But if you're writing to a fortran-convention file, you want this to go the other way
- In the file, one step in the **1st** index should jump you by 1, and the second by...

Your picture of the array

[2][0]	[2][1]	[2][2]	[2][3]
[1][0]	[1][1]	[1][2]	[1][3]
[0][0]	[0][1]	[0][2]	[0][3]

In memory

[0][0]	[0][1]	[0][2]	[0][3]	[1][0]	[1][1]	[1][2]	[1][3]	[2][0

Mapping memory space to file

- But if you're writing to a fortran-convention file, you want this to go the other way
- In the file, one step in the **1st** index should jump you by 1, and the second by **3**.
- The map you want is (1,3)

Your picture of the array

[2][0]	[2][1]	[2][2]	[2][3]
[1][0]	[1][1]	[1][2]	[1][3]
[0][0]	[0][1]	[0][2]	[0][3]

In memory

[0][0]	[0][1]	[0][2]	[0][3]	[1][0]	[1][1]	[1][2]	[1][3]	[2][0

Mapping memory space to file

Your picture of the array

[2][0]	[2][1]	[2][2]	[2][3]
[1][0]	[1][1]	[1][2]	[1][3]
[0][0]	[0][1]	[0][2]	[0][3]

```
start = count = stride = NULL;
int imap[2] = {1,3};

nc_put_varm_double(file_id,
dens_id, start, count, stride,
imap, data);


nf90_put_var(file_id, dens_id,
data, MAP=(/4,1/))
```

In memory

]	[0][1]	[0][2]	[0][3]	[1][0]	[1][1]	[1][2]	[1][3]	[2][0

More on NetCDF

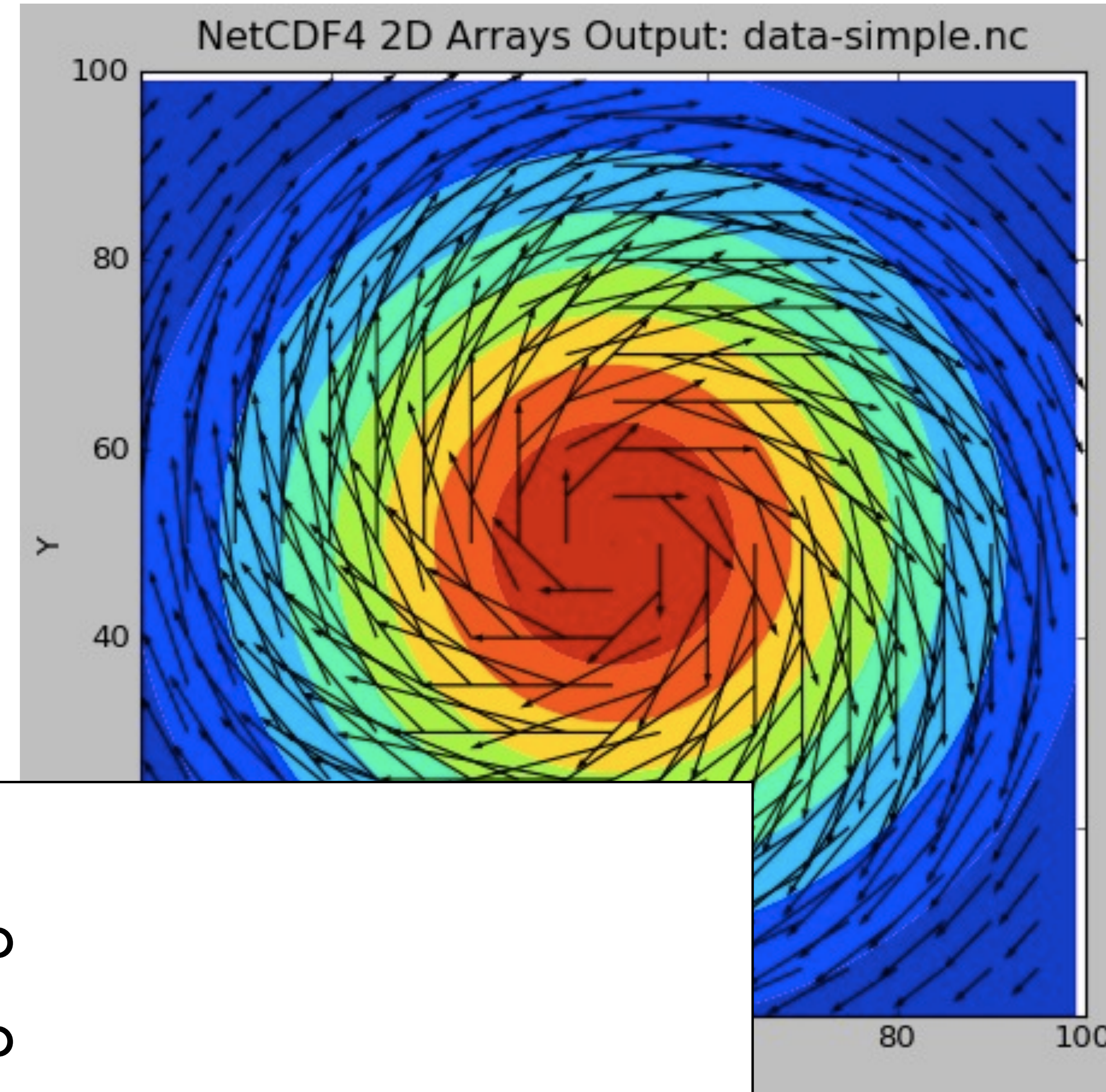
- http://www.unidata.ucar.edu/software/netcdf/
- Docs, mailing lists, tutorials, sample code, API, etc.

Sample Code

http://www.hdfgroup.org/HDF5/

```
$ cd parIO/hdf5

$ source /groups/h/hpc2011/bin/Parallel_IO.csh
$ make 2darray (C), or
$ make f2darray (F90)

$ ./{f,}2darray
$ ls *.h5

$ ../plots.py *.h5
```

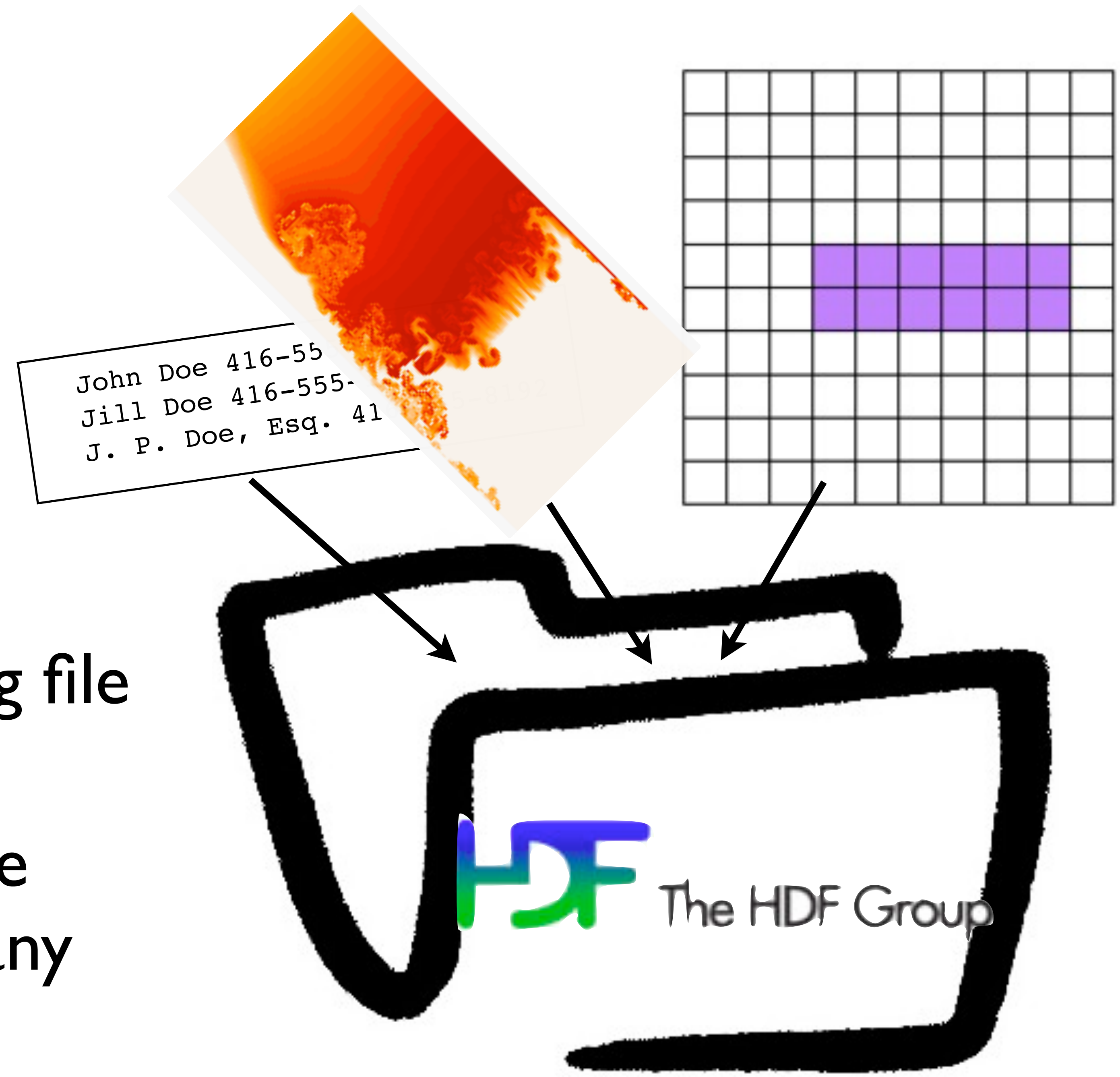
What is this .h5 file?



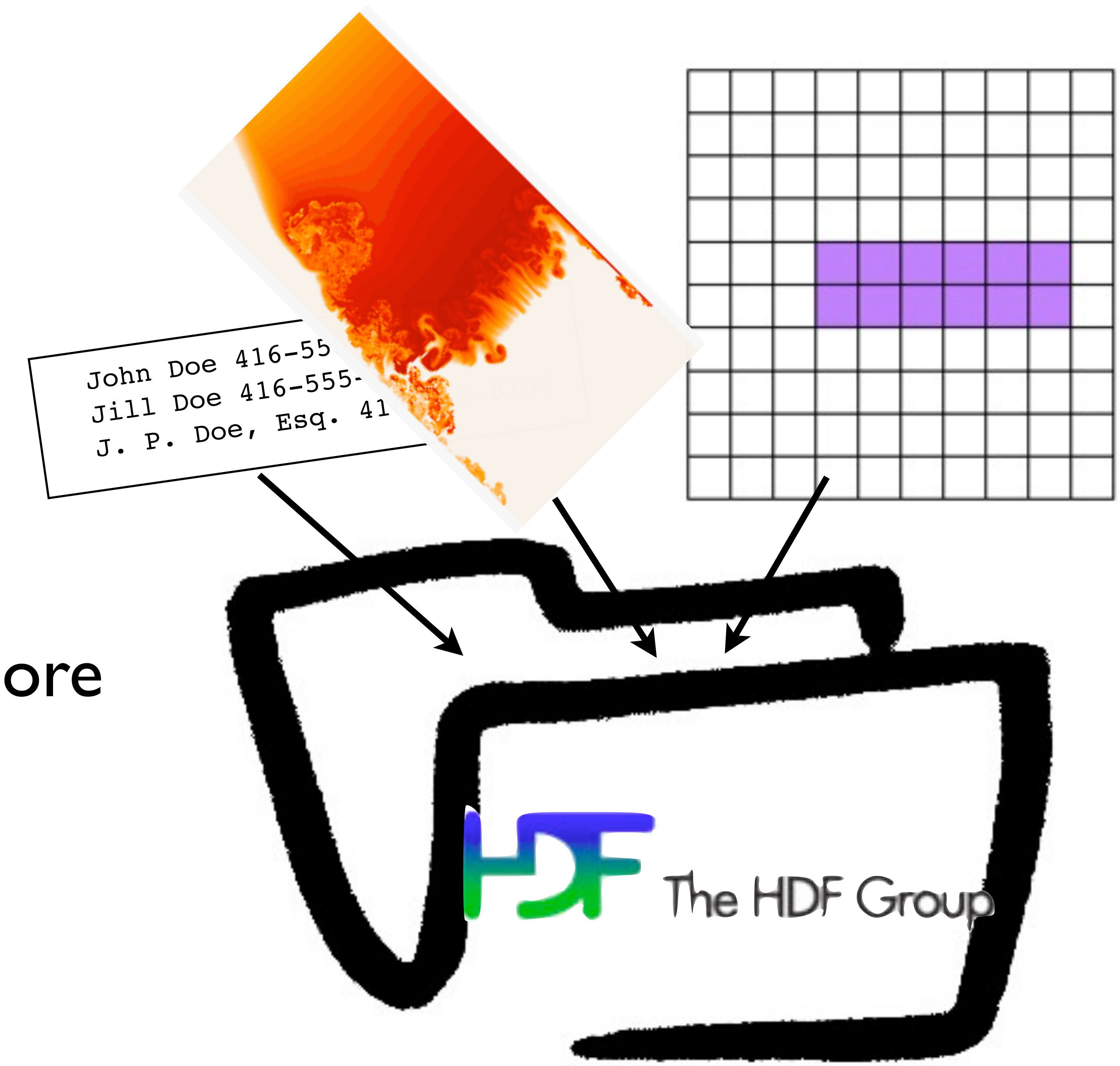

```
$ h5ls data-fort.h5
ArrayData                Group
OtherStuff               Group

$ h5ls data-fort.h5/ArrayData
dens                     Dataset {100, 100}
vel                      Dataset {100, 100, 2}
```

HDF5

- HDF5 is also self-describing file format and set of libraries
- Unlike NetCDF, much more general; can shove almost any type of data in there
- (We'll just be looking at large arrays, since that's our usual use case)



HDF5



- Much more general, and more low-level than NetCDF.
- (In fact, newest version of NetCDF implemented in HDF5).
- Pro: *can* do more!
- Con: **have** to do more.

2darray-simple.c

```
/* identifiers */
hid_t file_id, dens_dataset_id, vel_dataset_id;
hid_t dens_dataspace_id, vel_dataspace_id;

/* sizes */
hsize_t densdims[2], veldims[3];

/* status */
herr_t status;

/* Create a new file - truncate anything existing, use default properties
*/
file_id = H5Fcreate(rundata.filename, H5F_ACC_TRUNC, H5P_DEFAULT,
H5P_DEFAULT);

/* HDF5 routines generally return a negative number on failure.
 * Should check return values! */
if (file_id < 0) {
    fprintf(stderr,"Could not open file %s\n", rundata.filename);
    return;}
```

2darray-simple.c

```
/* identifiers */
hid_t file_id, dens_dataset_id, vel_dataset_id;
hid_t dens_dataspace_id, vel_dataspace_id;

/* sizes */
hsize_t densdims[2], veldims[3];

/* status */
herr_t status;

/* Create a new file - truncate anything
*/
file_id = H5Fcreate(rundata.filename, H5F_ACC_TRUNC, H5P_DEFAULT,
H5P_DEFAULT);

/* HDF5 routines generally return a negative number on failure.
 * Should check return values! */
if (file_id < 0) {
    fprintf(stderr,"Could not open file %s\n", rundata.filename);
    return;}
```

NetCDF used ints for everything - HDF5 distinguishes between ids, sizes, errors, uses its own types.

2darray-simple.c

```
/* identifiers */
hid_t file_id, dens_dataset_id, vel_dataset_id;
hid_t dens_dataspace_id, vel_dataspace_id;

/* sizes */
hsize_t densdims[2], veldims[3];

/* status */
herr_t status;

/* Create a new file - truncate anything existing, use default properties
*/
file_id = H5Fcreate(rundata.filename, H5F_ACC_TRUNC, H5P_DEFAULT,
H5P_DEFAULT);

/* HDF5 routines generally return a negative number on failure.
 * Should check return values! */
if (file_id < 0) {
    fprintf(stderr,"Could not open file %s\n", rundata.filename);
    return;}
```

H5F, H5P... ?

Decomposing the HDF5 API

- HDF5 API is large
- Constants, function calls start with H5x; x tells you what part of the library
- Table tells you (some) of those parts...
- Fortran the same, but usually end with _F

H5A	**A**ttributes
H5D	**D**atasets
H5E	**E**rrors
H5F	**F**iles
H5G	**G**roups
H5P	**P**roperties
H5S	Data **S**paces
H5T	Data **T**ypes

2darray-simple.c

```
/* Create the data space for the two datasets. */
densdims[0] = rundata.nx; densdims[1] = rundata.ny;
veldims[0] = 2; veldims[1] = rundata.nx; veldims[2] = rundata.ny;

dens_dataspace_id = H5Screate_simple(2, densdims, NULL);
vel_dataspace_id  = H5Screate_simple(3, veldims,  NULL);

/* Create the datasets within the file.
 * H5T_IEEE_F64LE is a standard (IEEE) double precision (64 bit)
 * floating (F) data type and will work on any machine.
 * H5T_NATIVE_DOUBLE would work too */

dens_dataset_id = H5Dcreate(file_id, "dens", H5T_IEEE_F64LE,
                                dens_dataspace_id, H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);

vel_dataset_id  = H5Dcreate(file_id, "vel",  H5T_IEEE_F64LE,
                                vel_dataspace_id,  H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
```

2darray-simple.c

```
/* Create the data space for the two datasets. */
densdims[0] = rundata.nx; densdims[1] = rundata.ny;
veldims[0] = 2; veldims[1] = rundata.nx; veldims[2] = rundata.ny;

dens_dataspace_id = H5Screate_simple(2, densdims, NULL);
vel_dataspace_id  = H5Screate_simple(3, veldims,  NULL);

/* Create the datasets within the file.
 * H5T_IEEE_F64LE is a standard (IEEE)
 * floating (F) data type and will work
 * H5T_NATIVE_DOUBLE would work too */

dens_dataset_id = H5Dcreate(file_id, "d
                                dens_da
                                H5P_DEF

vel_dataset_id  = H5Dcreate(file_id, "v
                                vel_dat
                                H5P_DEF
```

All data (in file or in mem) in HDF5 has a dataspace it lives in.

In NetCDF, just cartesian product of dimensions; here more general

2darray-simple.c

```
/* Create the data space for the two datasets. */
densdims[0] = rundata.nx; densdims[1] =
veldims[0] = 2; veldims[1] = rundata.nx

dens_dataspace_id = H5Screate_simple(2,
vel_dataspace_id  = H5Screate_simple(3,

/* Create the datasets within the file.
 * H5T_IEEE_F64LE is a standard (IEEE) 
 * floating (F) data type and will work
 * H5T_NATIVE_DOUBLE would work too */

dens_dataset_id = H5Dcreate(file_id, "dens", H5T_IEEE_F64LE,
                                dens_dataspace_id, H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);

vel_dataset_id  = H5Dcreate(file_id, "vel",  H5T_IEEE_F64LE,
                                vel_dataspace_id,  H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
```

Creating a data set like defining a variable in NetCDF.
Also declare the type you want it to be on disk.

2darray-simple.c

```
/* Write the data.  We're writing it from memory, where it is saved
 * in NATIVE_DOUBLE format */
status = H5Dwrite(dens_dataset_id, H5T_NATIVE_DOUBLE, H5S_ALL, H5S_ALL,
H5P_DEFAULT, &(dens[0][0]));
status = H5Dwrite(vel_dataset_id,  H5T_NATIVE_DOUBLE, H5S_ALL, H5S_ALL,
H5P_DEFAULT, &(vel[0][0][0]));


/* End access to groups & data sets and release resources used by them */
status = H5Sclose(dens_dataspace_id);
status = H5Dclose(dens_dataset_id);
status = H5Sclose(vel_dataspace_id);
status = H5Dclose(vel_dataset_id);


/* Close the file */
status = H5Fclose(file_id);
```

Write memory from all of memory to all of the dataset on the file. Values in mem are in the native double precision format.

2darray-simple.c

```
/* Write the data.  We're writing it from memory, where it is saved
 * in NATIVE_DOUBLE format */
status = H5Dwrite(dens_dataset_id, H5T_NATIVE_DOUBLE, H5S_ALL, H5S_ALL,
H5P_DEFAULT, &(dens[0][0]));
status = H5Dwrite(vel_dataset_id,  H5T_NATIVE_DOUBLE, H5S_ALL, H5S_ALL,
H5P_DEFAULT, &(vel[0][0][0]));


/* End access to groups & data sets and release resources used by them */
status = H5Sclose(dens_dataspace_id);
status = H5Dclose(dens_dataset_id);
status = H5Sclose(vel_dataspace_id);
status = H5Dclose(vel_dataset_id);


/* Close the file */
status = H5Fclose(file_id);
```

Close everything

f2darray-simple.f90

```
integer(hid_t) :: file_id
integer(hid_t) :: dens_space_id, vel_space_id
integer(hid_t) :: dens_id, vel_id
integer(hsize_t), dimension(2) :: densdims
integer(hsize_t), dimension(3) :: veldims

integer :: status

! first we have to open the FORTRAN inter
call h5open_f(status)

! create the file, check return code
call h5fcreate_f(rundata%filename, H5F_ACC_TRUNC_F, file_id, status)
if (status /= 0) then
    print *,'Could not open file ', rundata%filename
    return
endif
```

Fortran: values are integer(hid_t) or integer(hsize_t)

f2darray-simple.f90

```
integer(hid_t) :: file_id
integer(hid_t) :: dens_space_id, vel_space_id
integer(hid_t) :: dens_id, vel_id
integer(hsize_t), dimension(2) :: densdims
integer(hsize_t), dimension(3) :: veldims

integer :: status

! first we have to open the FORTRAN interface.
call h5open_f(status)

! create the file, check return code
call h5fcreate_f(rundata%filename, H5F_ACC_TRUNC_F, file_id, status)
if (status /= 0) then
    print *,'Could not open file ', rundata%filename
    return
endif
```

Have to start the FORTRAN interface

f2darray-simple.f90

```
integer(hid_t) :: file_id
integer(hid_t) :: dens_space_id, vel_space_id
integer(hid_t) :: dens_id, vel_id
integer(hsize_t), dimension(2) :: densdims
integer(hsize_t), dimension(3) :: veldims

integer :: status

! first we have to open the FORTRAN interface.
call h5open_f(status)

! create the file, check return code
call h5fcreate_f(rundata%filename, H5F_ACC_TRUNC_F, file_id, status)
if (status /= 0) then
    print *,'Could not open file ', rundata%filename
    return
endif
```

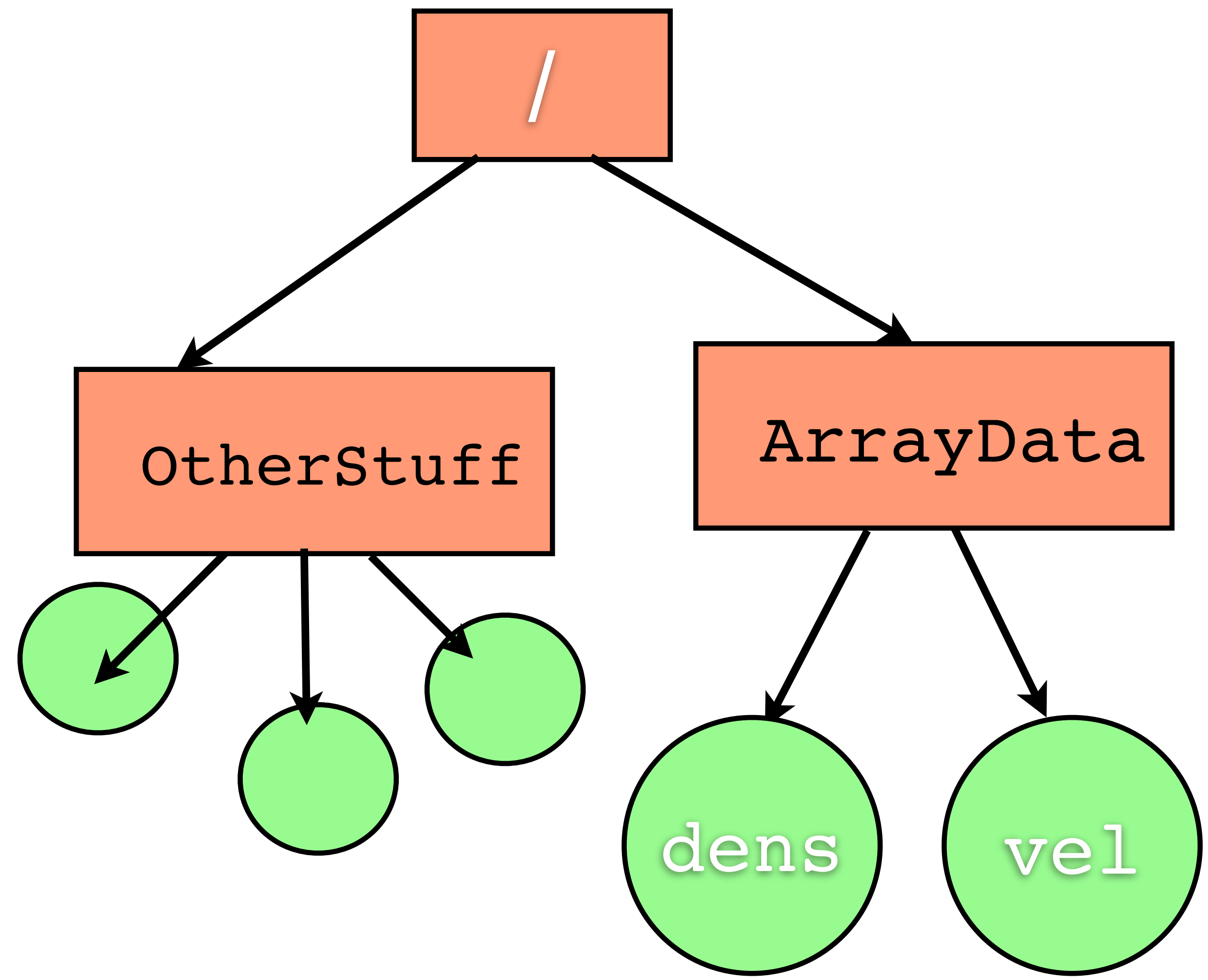
See what I mean about _F?

f2darray-simple.f90

```
! create the dataspaces corresponding to our variables
densdims = (/ rundata % nx, rundata % ny /)
call h5screate_simple_f(2, densdims, dens_space_id, status)

veldims = (/ 2, rundata % nx, rundata % ny /)
call h5screate_simple_f(3, veldims, vel_space_id, status)

! now that the dataspaces are defined, we can define variables on them

call h5dcreate_f(file_id, "dens", H5T_IEEE_F64LE, dens_space_id, dens_id,
status)
call h5dcreate_f(file_id, "vel" , H5T_IEEE_F64LE, vel_space_id,  vel_id,
status)
```

In F90 interface, a lot of less-common arguments are optional; fewer H5P_DEFAULTs kicking around

HDF5 Groups



- HDF5 has a structure a bit like a unix filesystem:
- "Groups" - directories
- "Datasets" - files
- NetCDF4 now has these, but breaks compatibility with NetCDF3 files

2darray.c

```
/* Create a new group within the new file */
arr_group_id = H5Gcreate(file_id,"/ArrayData", H5P_DEFAULT, H5P_DEFAULT,
H5P_DEFAULT);
...

dens_dataset_id = H5Dcreate(file_id, "/ArrayData/dens", H5T_IEEE_F64LE,
                                dens_dataspace_id, H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
vel_dataset_id  = H5Dcreate(file_id, "/ArrayData/vel",  H5T_IEEE_F64LE,
                                vel_dataspace_id,  H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
```

Can specify that a dataset goes in a group by giving it an "absolute path"...

```
/* Create a new group within the new file */
arr_group_id = H5Gcreate(file_id,"/ArrayData", H5P_DEFAULT, H5P_DEFAULT,
H5P_DEFAULT);
...

dens_dataset_id = H5Dcreate(arr_group_id, "dens", H5T_IEEE_F64LE,
                                dens_dataspace_id, H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
vel_dataset_id  = H5Dcreate(arr_group_id, "vel",  H5T_IEEE_F64LE,
                                vel_dataspace_id,  H5P_DEFAULT,
                                H5P_DEFAULT, H5P_DEFAULT);
```

...or just by creating it *in* the group, rather than the file.

What NetCDF, HDF *aren't*

- Databases
- Seem like - lots of information, in key value pairs.
- Relational databases - interrelated tables of **small** pieces of data
- Very easy/fast to query
- But can't do subarrays, etc..

Books

bid	title	isbn	author	date	volume
1	Big Cats	24589673-0	Cat, Simon	2003	2
2	Plants	24316759-1	Smith, Rose	1967	1
3	Sailing	34817645-0	Jones, Tom	1868	1

Transactions

tid	date	bid	pid	duedate	
1	02/11/08	3	2	16/11/08	
2	04/11/08	1	3	18/11/08	

Borrowers

pid	firstname	lastname	address	phone	fines
1	Fred	Thompson	2 Reach Rd.	827-9867	2.25
2	Sam	Trunker	23 stone St.	243-0955	0
3	Tony	Sanchas	4 two Rd.	123-6453	0

Databases for science

```
INSERT INTO benchmarkruns
values (newrunnum, datestr,
timestr, juliannum)

...
SELECT nprocs, test, size,
transport, mpitype, runtime,
mopsperproc, run FROM
mpirundata WHERE (success=1)
```

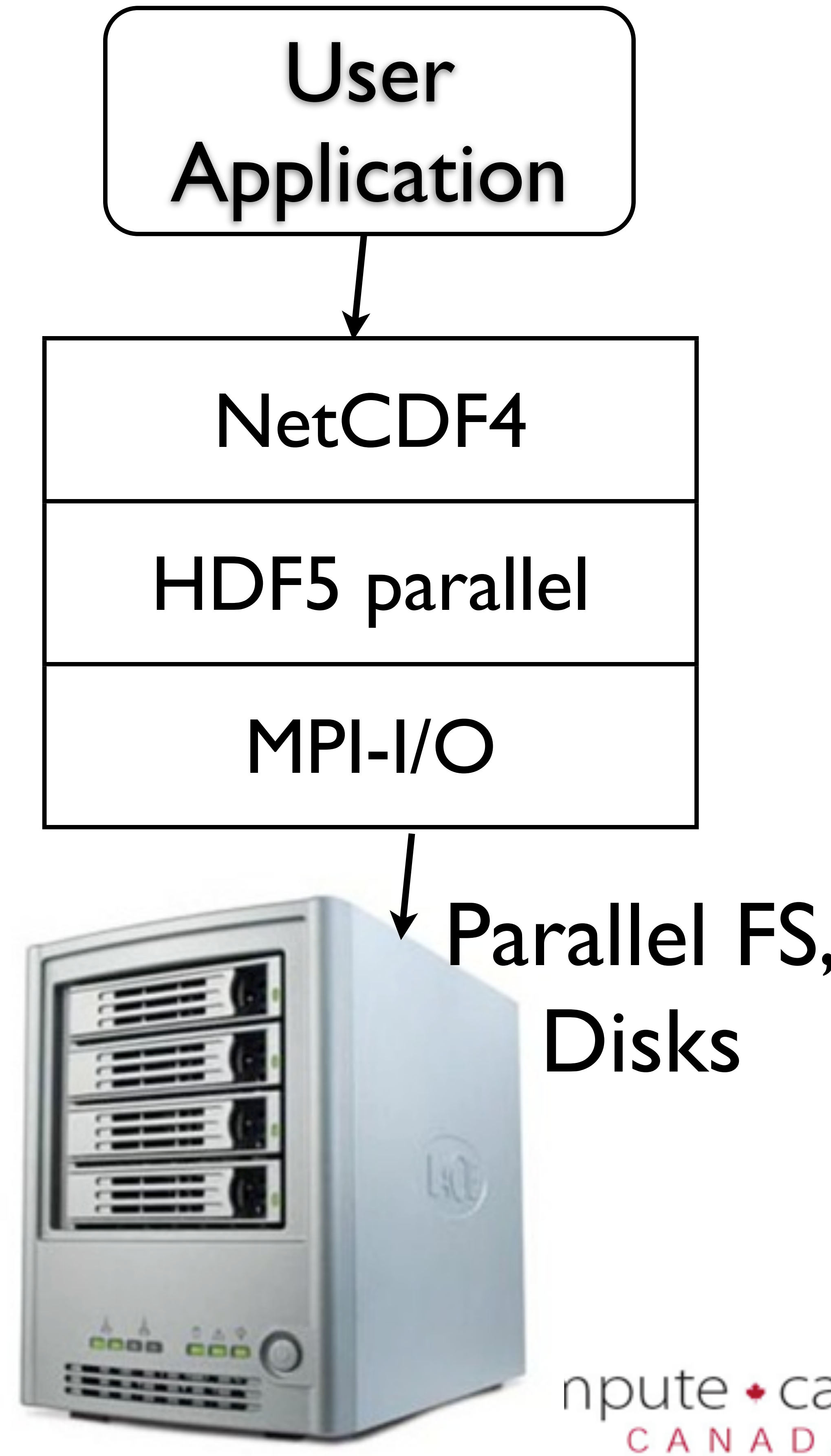
run#	success	size	transport	...
93	no	12k	eth	
1	yes	512	eth	
87	yes	64	ib	
13	no	32	eth	

...

Parallel I/O using NetCDF4, HDF5

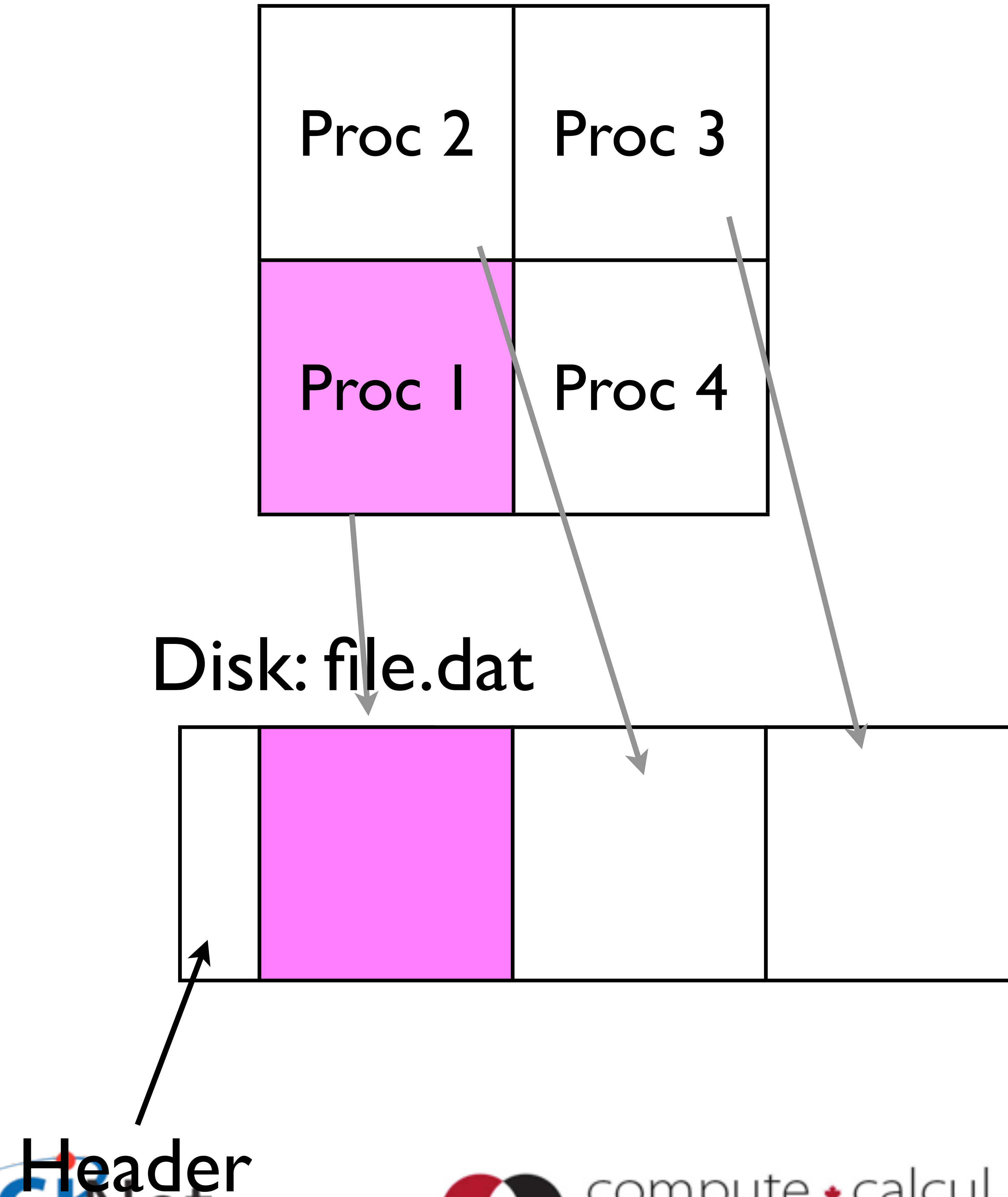
Parallel I/O libraries

- Can use the same NetCDF(4), HDF5 libraries to do Parallel IO on top of the MPI-I/O library
- Reading file afterwards, can't tell the difference.
- Fairly minor differences in function calls to do parallel I/O
- Hard part is figuring out what/ where to write



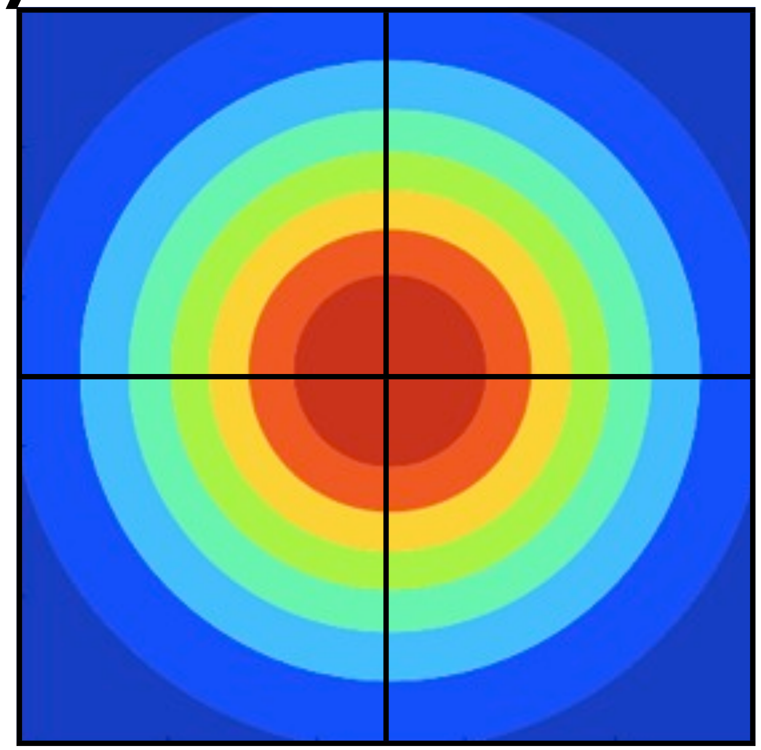
Parallel IO to One file

- Can be made to work efficiently, but must write to *disjoint* chunks of file
- Should write *big* disjoint chunks of file.



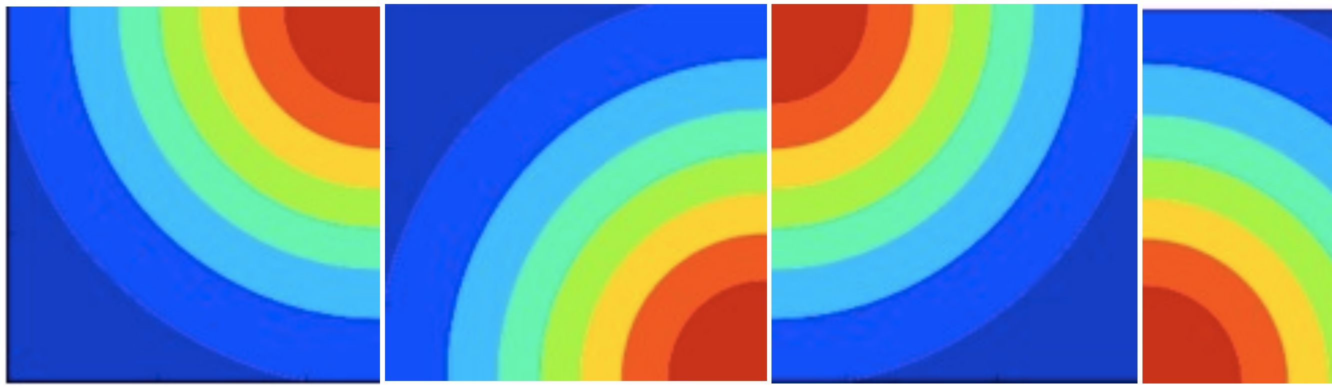
How do you decide where to write?

Memory:



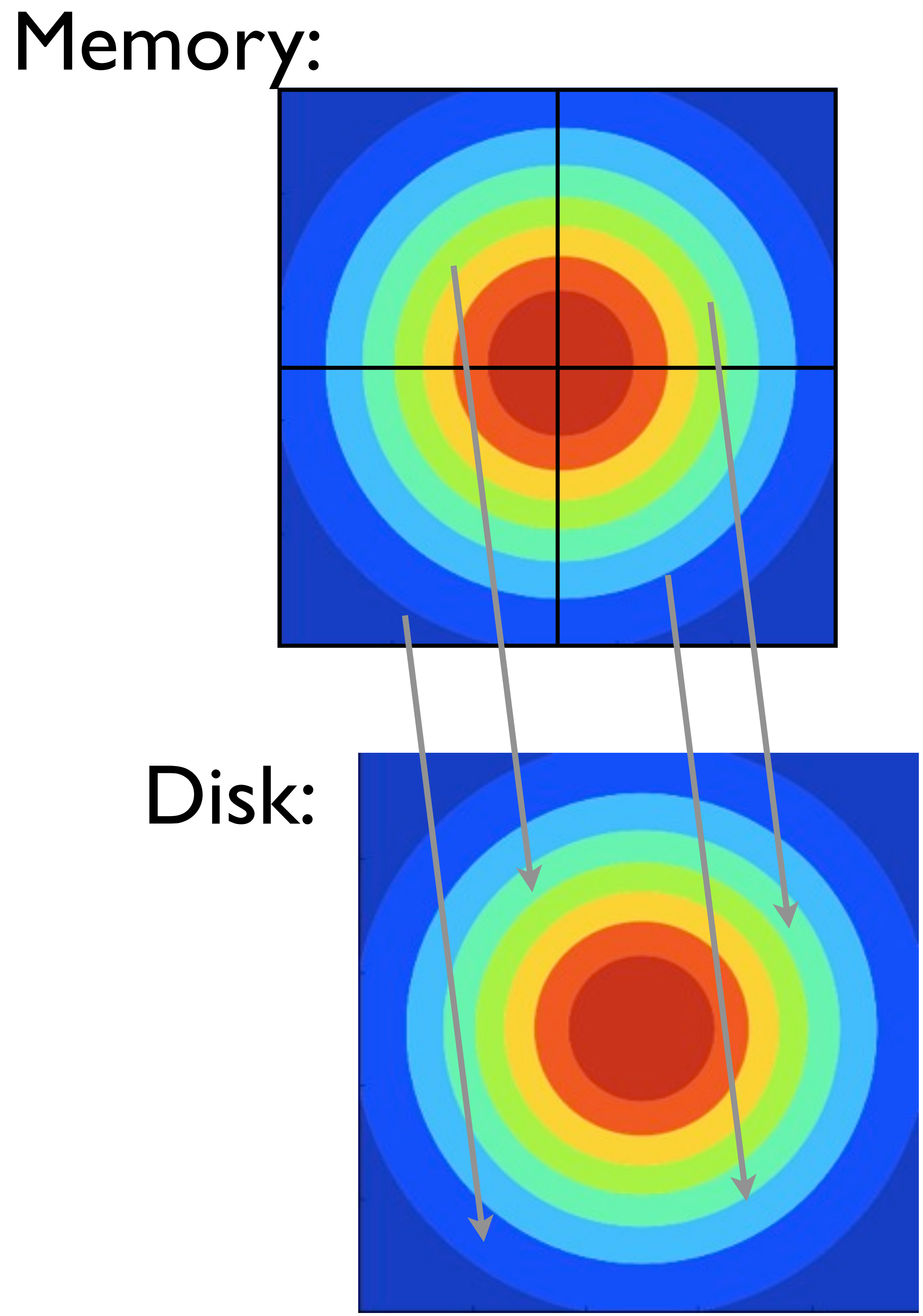
- One possibility: each processor writes out its part of problem, in order.
- Pros - can be super fast.
- Cons - Output depends on number of processors run on. Analysis routines, restarts...

Disk:

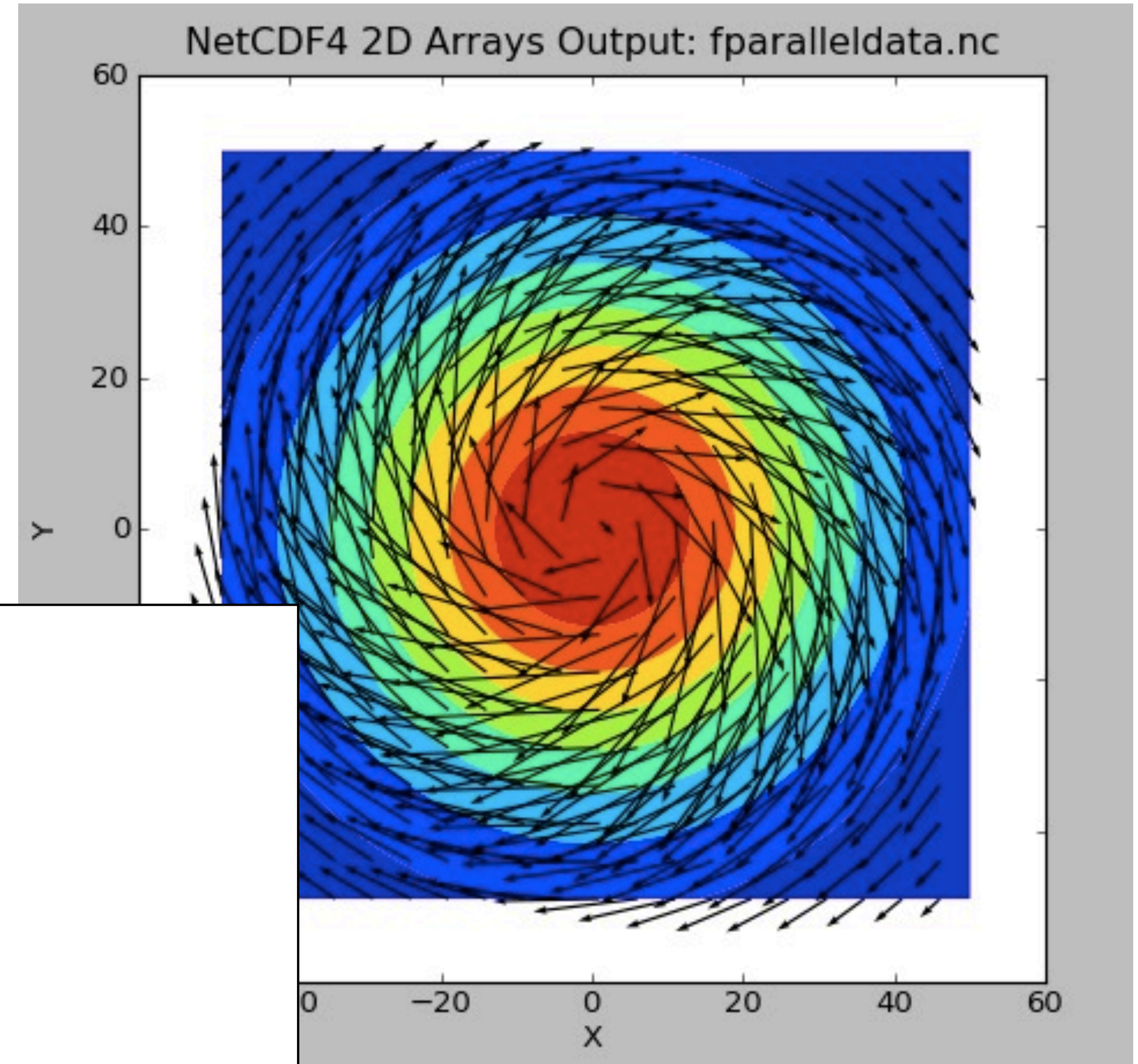


How do you decide where to write?

- Other possibility: Write out chunks as they would be in memory on serial machine
- Pros: File looks the same no matter how many processes were used to write.
- Cons: Noncontig access; may be slower, but MPI-IO collective + good parallel FS should make competitive.



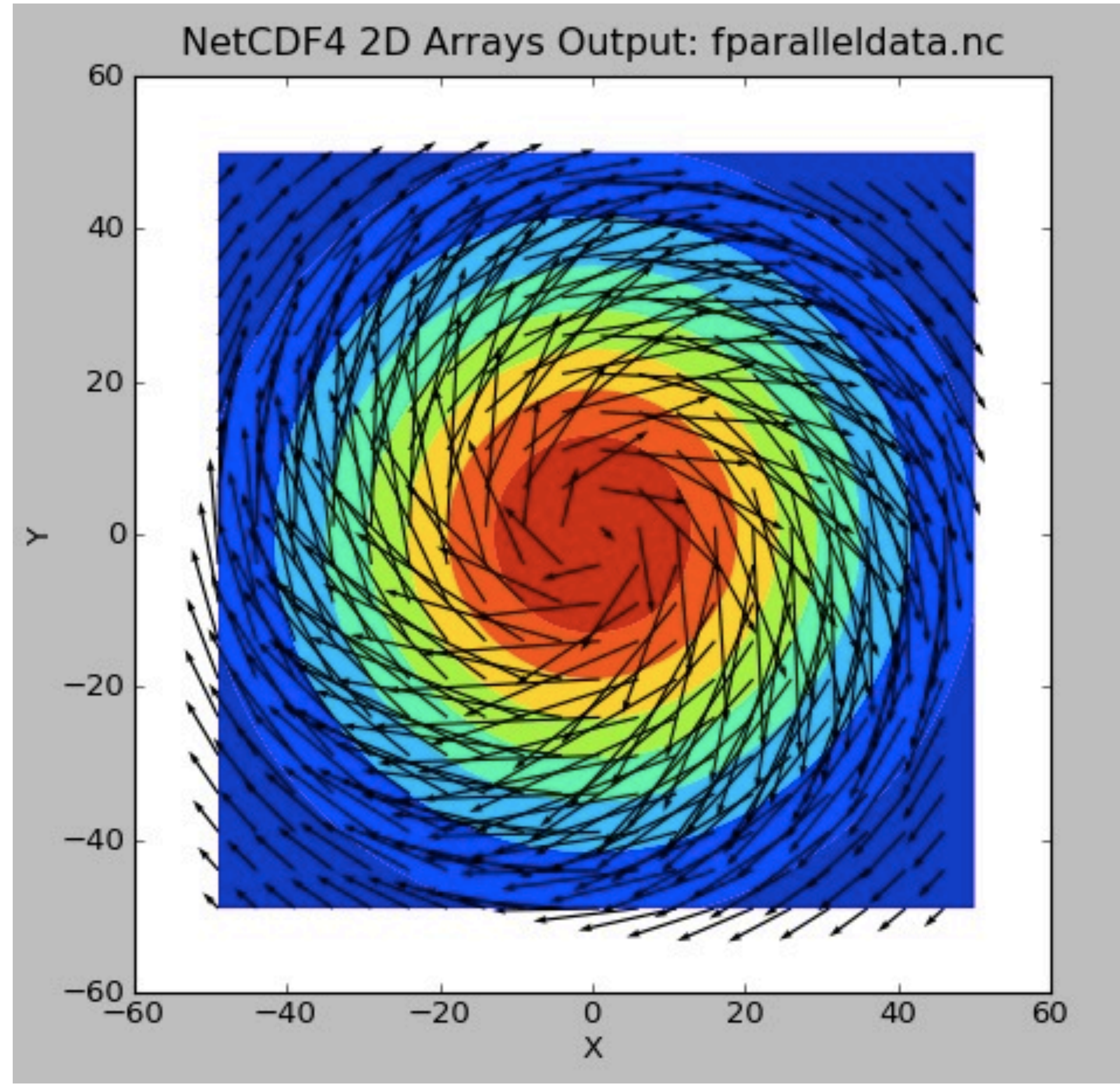
Sample Code



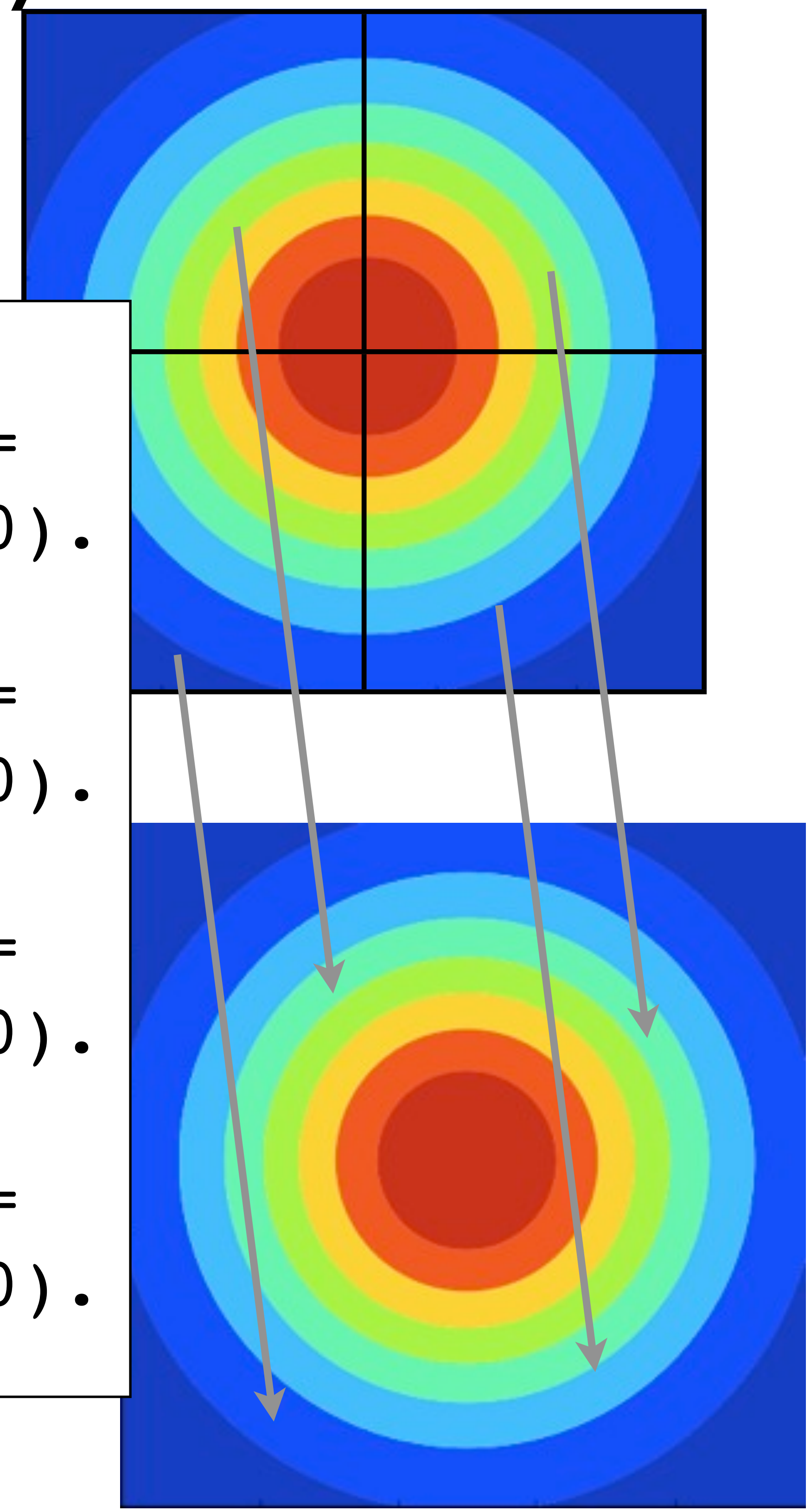

```
$ cd
$ cd parIO/netcdf

$ make parallel2darray (C), or
$ make fparallel2darray (F90)

$ mpirun -np 4 parallel2darray

$ ls *.nc
$ source ../seriallibs
$ ../plots.py paralleldata.nc
```

Sample Code

- Can do an ncdump -h...
- No trace of being written by different files
- Looks the same; code to read in is identical
- And not that much harder to code!
- By far the trickiest part is figuring out where in the file to write.



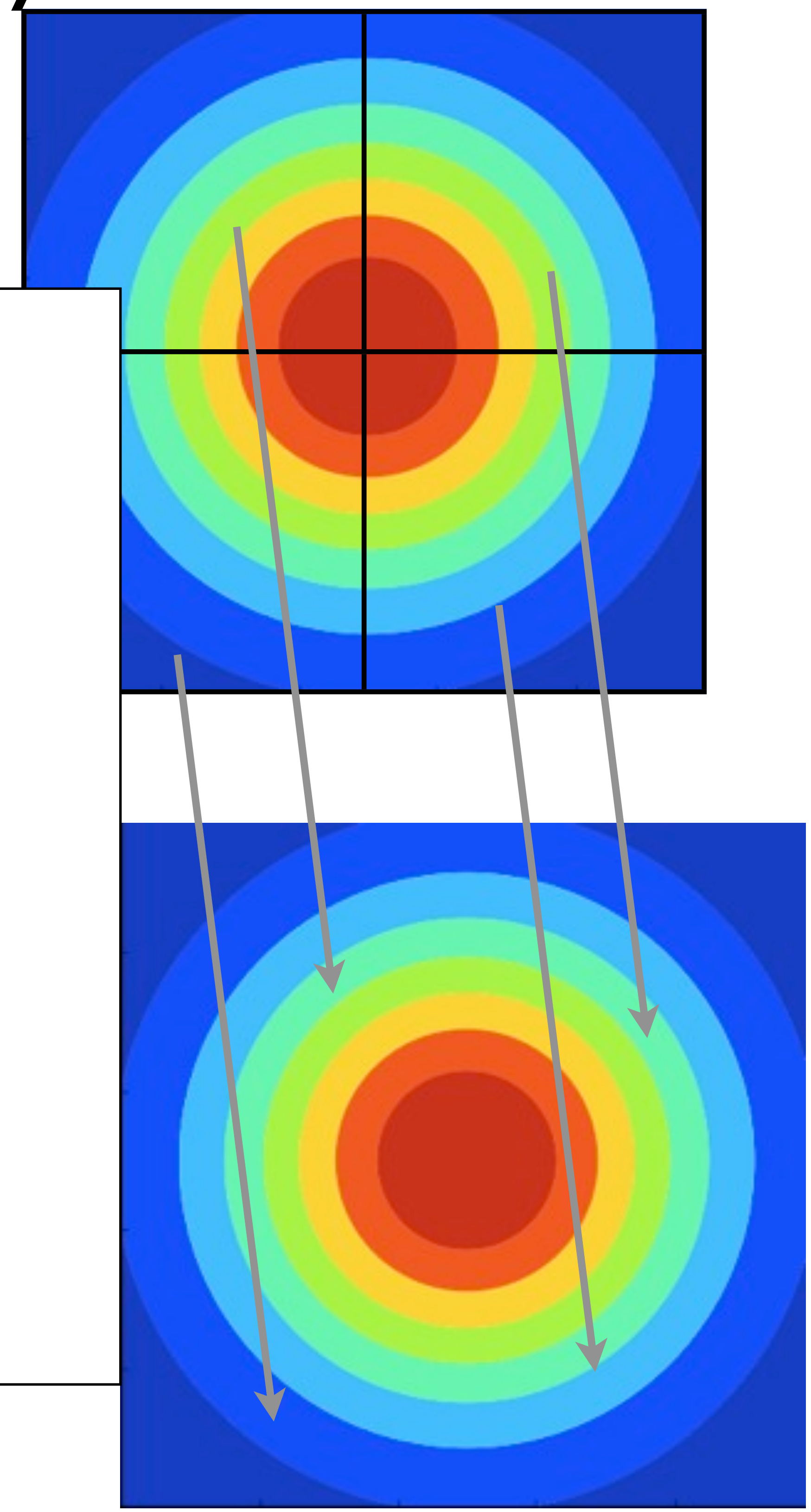
Memory:



```
$ mpirun -np 4 ./fparallel2darray
[   0] gets ( 0,   0): local points =
( 50, 50); global points = (100,100).

[   1] gets ( 1,   0): local points =
( 50, 50); global points = (100,100).

[   2] gets ( 0,   1): local points =
( 50, 50); global points = (100,100).

[   3] gets ( 1,   1): local points =
( 50, 50); global points = (100,100).
```

Memory:

```
[   0]: denstarts, denscounts
        =    1    1   50   50
[   1]: denstarts, denscounts
        =   51    1   50   50
[   2]: denstarts, denscounts
        =    1   51   50   50
[   3]: denstarts, denscounts
        =   51   51   50   50
```



fparallel2darray.f90

```
call MPI_Info_create(info, status)
call MPI_Info_set(info,"IBM_largeblock_io","true", status)

mode_flag = IOR(NF90_MPIIO, NF90_CLOBBER)
mode_flag = IOR(mode_flag, NF90_NETCDF4)
status = nf90_create_par(rundata%filename, mode_flag,
MPI_COMM_WORLD, info, file_id)
if (status /= NF90_NOERR) then
      print *,'Could not open file ', rundata%filename
      return
endif
```

fparallel2darray.f90

```
call MPI_Info_create(info, status)
call MPI_Info_set(info,"IBM_largeblock_io","true", status)

mode_flag = IOR(NF90_MPIIO, NF90_CLOBBER)
mode_flag = IOR(mode_flag, NF90_NETCDF4)
status = nf90_create_par(rundata%filename, mode_flag,
MPI_COMM_WORLD, info, file_id)
if (status /= NF90_NOERR) then
      print *,'Could not open file ', rundata%filename
      return
endif
```

create_par rather than create

fparallel2darray.f90

```
call MPI_Info_create(info, status)
call MPI_Info_set(info,"IBM_largeblock_io","true", status)

mode_flag = IOR(NF90_MPIIO, NF90_CLOBBER)
mode_flag = IOR(mode_flag, NF90_NETCDF4)
status = nf90_create_par(rundata%filename, mode_flag,
MPI_COMM_WORLD, info, file_id)
if (status /= NF90_NOERR) then
      print *,'Could not open file ', rundata%filename
      return
endif
```

mode_flag = CLOBBER | MPIIO | NETCDF4

fparallel2darray.f90

```
call MPI_Info_create(info, status)
call MPI_Info_set(info,"IBM_largeblock_io","true", status)

mode_flag = IOR(NF90_MPIIO, NF90_CLOBBER)
mode_flag = IOR(mode_flag, NF90_NETCDF4)
status = nf90_create_par(rundata%filename, mode_flag,
MPI_COMM_WORLD, info, file_id)
if (status /= NF90_NOERR) then
      print *,'Could not open file ', rundata%filename
      return
endif
```

Extra arguments: communicator that will do the I/O

fparallel2darray.f90

```
call MPI_Info_create(info, status)
call MPI_Info_set(info,"IBM_largeblock_io","true", status)

mode_flag = IOR(NF90_MPIIO, NF90_CLOBBER)
mode_flag = IOR(mode_flag, NF90_NETCDF4)
status = nf90_create_par(rundata%filename, mode_flag,
MPI_COMM_WORLD, info, file_id)
if (status /= NF90_NOERR) then
      print *,'Could not open file ', rundata%filename
      return
endif
```

Extra arguments: MPI Info; can pass MPI-I/O "hints"

fparallel2darray.f90

```
status = nf90_def_dim(file_id, 'X', rundata%globalnx, xdim_id)
status = nf90_def_dim(file_id, 'Y', rundata%globalny, ydim_id)
status = nf90_def_dim(file_id, 'velocity components', 2,
vcomp_id)

! now that the dimensions are defined, define variables

densdims = (/ xdim_id, ydim_id /)
veldims = (/ vcomp_id, xdim_id, ydim_id /)

status = nf90_def_var(file_id, 'Density',  NF90_DOUBLE, densdims,
dens_id)
status = nf90_def_var(file_id, 'Velocity', NF90_DOUBLE, veldims,
vel_id)
```

Defining variables identical (but global v local)

fparallel2darray.f90

```
status = nf90_var_par_access(file_id, dens_id, NF90_COLLECTIVE)
status = nf90_var_par_access(file_id, vel_id,  NF90_COLLECTIVE)


status = nf90_put_var(file_id, dens_id, dens, start=densstarts,
count=denscounts)
status = nf90_put_var(file_id, vel_id,  vel, start=velstarts,
count=velcounts)


status = nf90_close(file_id)
```

Define how we'll be accessing *variables* - COLLECTIVE vs INDEPENDANT. (eg, Write_all vs. Write).

fparallel2darray.f90

```
status = nf90_var_par_access(file_id, dens_id, NF90_COLLECTIVE)
status = nf90_var_par_access(file_id, vel_id,  NF90_COLLECTIVE)


status = nf90_put_var(file_id, dens_id, dens, start=densstarts,
count=denscounts)
status = nf90_put_var(file_id, vel_id,  vel, start=velstarts,
count=velcounts)


status = nf90_close(file_id)
```

put_var is exactly like serial with subsections - starts, counts

fparallel2darray.f90

```
status = nf90_var_par_access(file_id, dens_id, NF90_COLLECTIVE)
status = nf90_var_par_access(file_id, vel_id,  NF90_COLLECTIVE)


status = nf90_put_var(file_id, dens_id, dens, start=densstarts,
count=denscounts)
status = nf90_put_var(file_id, vel_id,  vel, start=velstarts,
count=velcounts)


status = nf90_close(file_id)
```

close is the same as ever.

serial.c

```c
/* name of units for dens, vel */
const char *densunit="g/cm^3";
const char *velunit="cm/s";



/* return status */
int status;


/* set up x, y coordinates */
x = (float *)malloc(rundata.nx * sizeof(float));
y = (float *)malloc(rundata.ny * sizeof(float));
for (i=0; i<rundata.nx; i++)
    x[i] = (1.*i-rundata.nx/2.);
for (i=0; i<rundata.ny; i++)
    y[i] = (1.*i-rundata.ny/2.);




/* Create a new file - clobber anything existing */
status = nc_create(rundata.filename, NC_CLOBBER, &file_id);

/* netCDF routines return NC_NOERR on success */
if (status != NC_NOERR) {
    fprintf(stderr,"Could not open file %s\n", rundata.filename);
    return;
}

/* define the dimensions */
nc_def_dim(file_id, "X", rundata.nx, &xdim_id);
nc_def_dim(file_id, "Y", rundata.ny, &ydim_id);
nc_def_dim(file_id, "velocity component", 2, &vcomp_id);

/* define the coordinate variables,... */
```

parallel.c

```c
/* name of units for dens, vel */
const char *densunit="g/cm^3";
const char *velunit="cm/s";

/* offsets for sub-regions of arrays */
size_t starts[3];
size_t counts[3];

/* return status */
int status;

/* MPI-IO hints for performance */
MPI_Info info;

/* set up x, y coordinates */
x = (float *)malloc(rundata.globalnx * sizeof(float));
y = (float *)malloc(rundata.globalny * sizeof(float));
for (i=0; i<rundata.globalnx; i++)
    x[i] = (1.*i-rundata.globalnx/2.);
for (i=0; i<rundata.globalny; i++)
    y[i] = (1.*i-rundata.globalny/2.);


/* set the MPI-IO hints for better performance on GPFS */
MPI_Info_create(&info);
MPI_Info_set(info,"IBM_largeblock_io","true");

/* Create a new file - clobber anything existing */
status = nc_create_par(rundata.filename, NC_MPIIO|NC_CLOBBER|N
                       MPI_COMM_WORLD, info, &file_id);
/* netCDF routines return NC_NOERR on success */
if (status != NC_NOERR) {
    fprintf(stderr,"Could not open file %s\n", rundata.filenam
    return;
}

/* define the dimensions */
nc_def_dim(file_id, "X", rundata.globalnx, &xdim_id);
nc_def_dim(file_id, "Y", rundata.globalny, &ydim_id);
nc_def_dim(file_id, "velocity component", 2, &vcomp_id);

/* define the coordinate variables,... */
```

serial.c

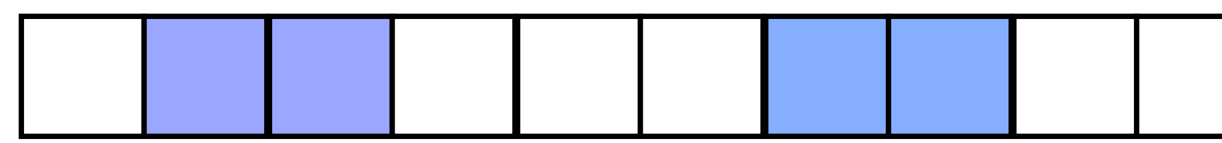
```
nc_def_var(file_id, "Density",  NC_DOUBLE, 2, densdims, &dens_id);
nc_def_var(file_id, "Velocity", NC_DOUBLE, 3, veldims,  &vel_id);

/* assign units to the variables */
nc_put_att_text(file_id, dens_id, "units", strlen(densunit), densunit);
nc_put_att_text(file_id, vel_id,  "units", strlen(velunit),  velunit);

/* we are now done defining variables and their attributes */
nc_enddef(file_id);

/* Write out the data to the variables we've defined */
nc_put_var_float(file_id, xcoord_id, x);
nc_put_var_float(file_id, ycoord_id, y);

nc_put_var_double(file_id, dens_id, &(dens[0][0]));
nc_put_var_double(file_id, vel_id,  &(vel[0][0][0]));

nc_close(file_id);
return;
```

parallel.c

```
nc_def_var(file_id, "Density",  NC_DOUBLE, 2, densdims, &dens_id)
nc_def_var(file_id, "Velocity", NC_DOUBLE, 3, veldims,  &vel_id);

/* assign units to the variables */
nc_put_att_text(file_id, dens_id, "units", strlen(densunit), dens
nc_put_att_text(file_id, vel_id,  "units", strlen(velunit),  velu

/* we are now done defining variables and their attributes */
nc_enddef(file_id);

/* Write out the data to the variables we've defined */
nc_put_var_float(file_id, xcoord_id, x);
nc_put_var_float(file_id, ycoord_id, y);

/* The big data will be written to collectively;
 * the alternative is NC_INDEPENDENT  */
nc_var_par_access(file_id, dens_id, NC_COLLECTIVE);
nc_var_par_access(file_id, vel_id,  NC_COLLECTIVE);

/* densities */
starts[0] = (rundata.globalnx/rundata.npx)*rundata.myx;
starts[1] = (rundata.globalny/rundata.npy)*rundata.myy;
counts[0]  = rundata.localnx;
counts[1]  = rundata.localny;

nc_put_vara_double(file_id, dens_id, starts, counts, &(dens[0][0]

/* velocities */
starts[0] = 0;
starts[1] = (rundata.globalnx/rundata.npx)*rundata.myx;
starts[2] = (rundata.globalny/rundata.npy)*rundata.myy;
counts[0] = 2;
counts[1] = rundata.localnx;
counts[2] = rundata.localny;

nc_put_vara_double(file_id, vel_id, starts, counts, &(vel[0][0][0

nc_close(file_id);
return;
}
```

HDF5 Hyperslabs

- Parallel HDF5 similar to parallel NetCDF - fairly modest changes to structure of code
- Different (more low-level, natch) way of dealing with sub-regions
- Offset, block, count, stride



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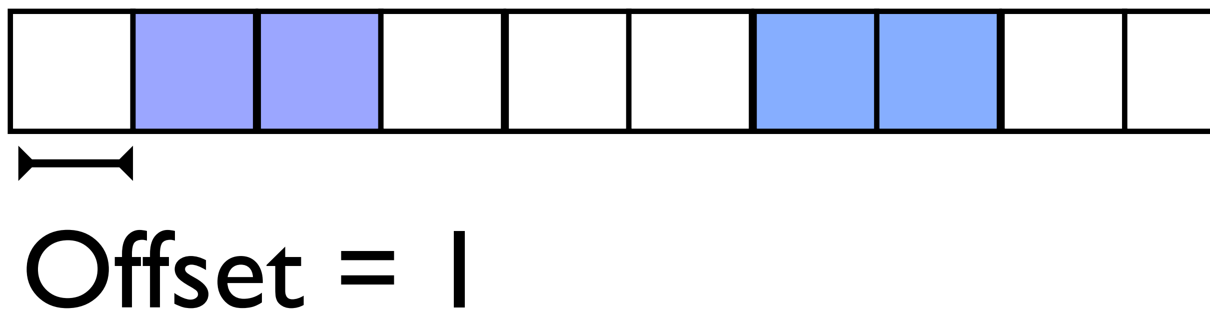

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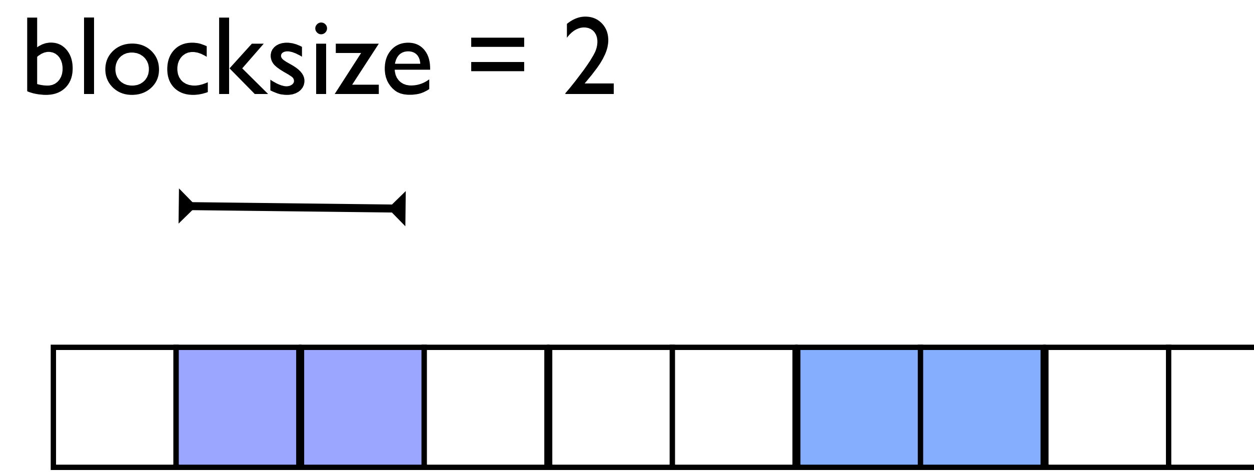
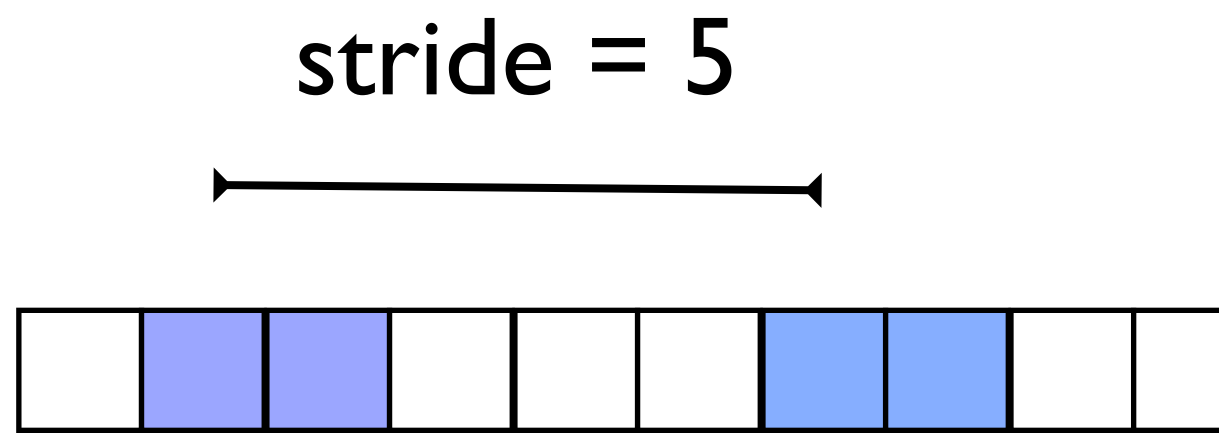


HDF5 Hyperslabs



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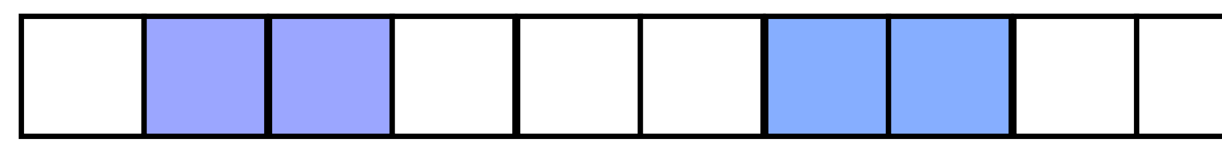
HDF5 Hyperslabs

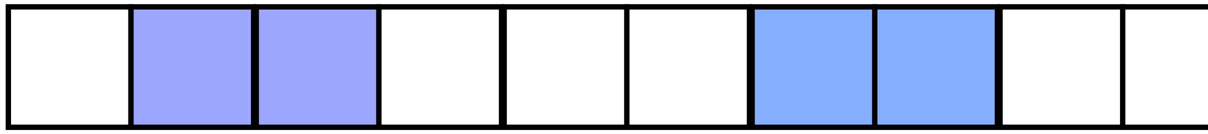
- Parallel HDF5 similar to parallel NetCDF - fairly modest changes to structure of code
- Different (more low-level, natch) way of dealing with sub-regions
- Offset, block, count, stride
- (MPI_Type_vector)

count = 2



HDF5 Hyperslabs

count = 2



- Parallel HDF5 similar to parallel NetCDF - fairly modest changes to structure of code
- Different (more low-level, natch) way of dealing with sub-regions
- Offset, block, count, stride
- Hyperslab - one of these per dimensions.
- (offset,block) just like (start, counts) in netcdf.

parallel2darray.c

```
/* set the MPI-IO hints for better performance on GPFS */
MPI_Info_create(&info);
MPI_Info_set(info,"IBM_largeblock_io","true");

/* Set up the parallel environment for file access*/
fap_id = H5Pcreate(H5P_FILE_ACCESS);
/* Include the file access property with IBM hint */
H5Pset_fapl_mpio(fap_id, MPI_COMM_WORLD, info);

/* Set up the parallel environment */
dist_id = H5Pcreate(H5P_DATASET_XFER);
/* we'll be writing collectively */
H5Pset_dxpl_mpio(dist_id, H5FD_MPIO_COLLECTIVE);
```

parallel2darray.c

```
/* set the MPI-IO hints for better performance on GPFS */
MPI_Info_create(&info);
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/* Set up the parallel environment */
dist_id = H5Pcreate(H5P_DATASET_XFER);
/* we'll be writing collectively */
H5Pset_dxpl_mpio(dist_id, H5FD_MPIO_COLLECTIVE);
```

Same as NetCDF; this is a property of the *file*

parallel2darray.c

```
/* set the MPI-IO hints for better performance on GPFS */
MPI_Info_create(&info);
MPI_Info_set(info,"IBM_largeblock_io","true");

/* Set up the parallel environment for file access*/
fap_id = H5Pcreate(H5P_FILE_ACCESS);
/* Include the file access property with IBM hint */
H5Pset_fapl_mpio(fap_id, MPI_COMM_WORLD, info);

/* Set up the parallel environment */
dist_id = H5Pcreate(H5P_DATASET_XFER);
/* we'll be writing collectively */
H5Pset_dxpl_mpio(dist_id, H5FD_MPIO_COLLECTIVE);
```

Collective/independant: this is a property of accessing a *variable*

parallel2darray.c

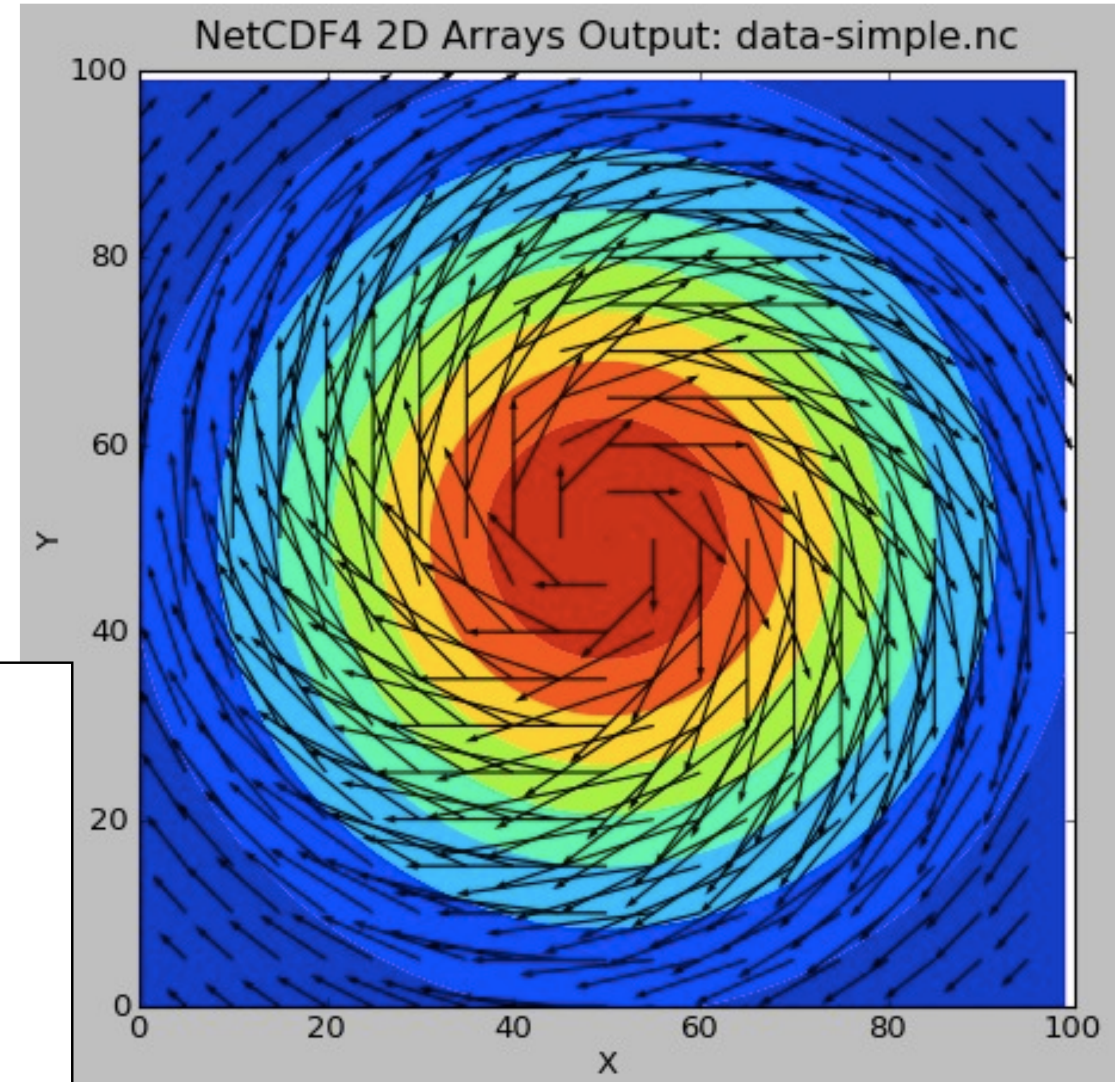
```
offsets[0] = (rundata.globalnx/rundata.npx)*rundata.myx;
offsets[1] = (rundata.globalny/rundata.npy)*rundata.myy;
blocks[0]  = rundata.localnx;
strides[0] = strides[1] = 1;
counts[0] = counts[1] = 1;


globaldensspace = H5Dget_space(dens_dataset_id);
H5Sselect_hyperslab(globaldensspace,H5S_SELECT_SET, offsets,
strides, counts, blocks);


status = H5Dwrite(dens_dataset_id, H5T_NATIVE_DOUBLE,
loc_dens_dataspace_id, globaldensspace, dist_id, &(dens[0]
[0]));
```

Select hyperslab, and write; parallelism is in distribution_id

Projects




```
$ cd parIO/hydro{c,f}
```

Write hdf5, netcdf outputs

```
$ cd parIO/hydro{c,f}-mpi
```

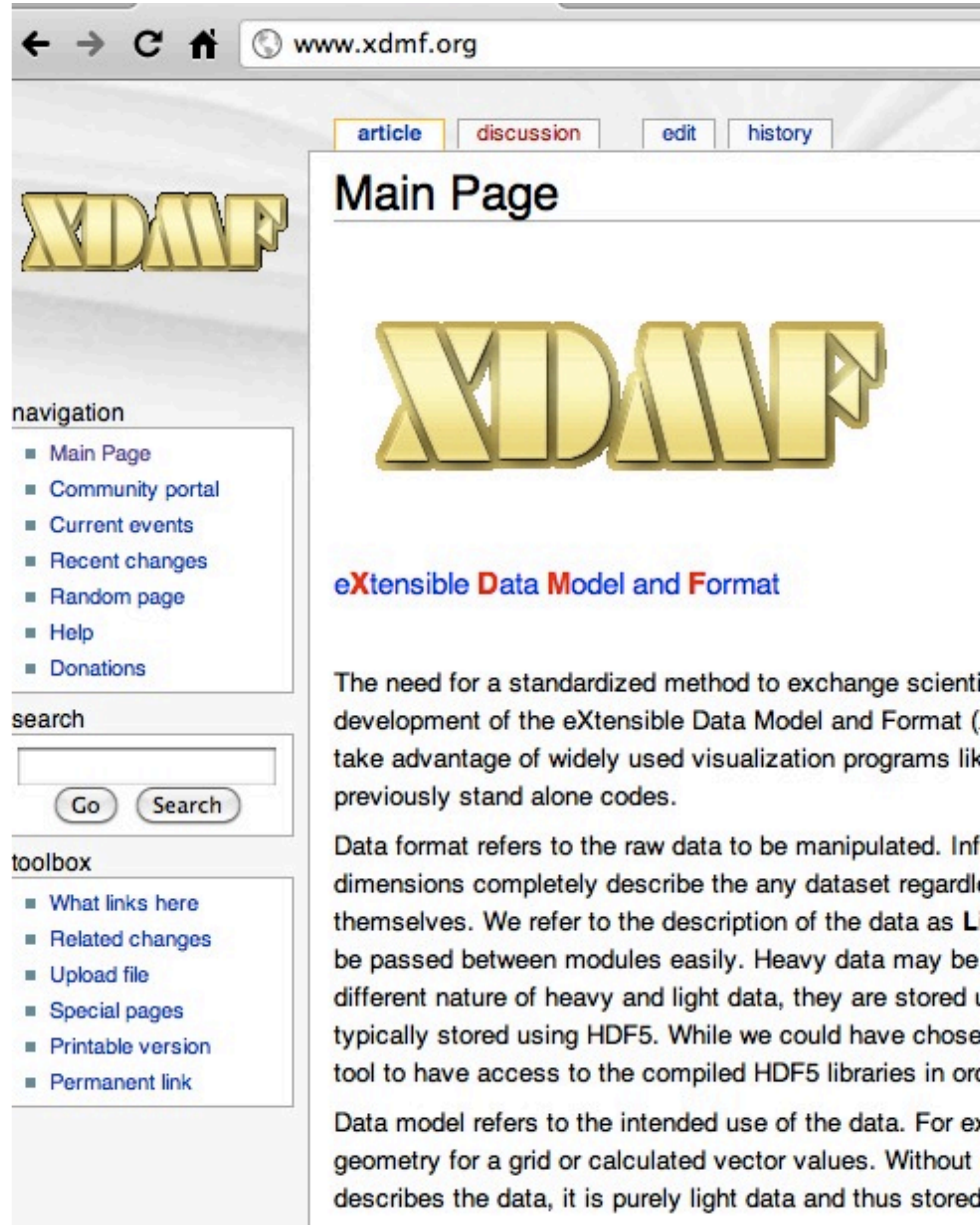
Write ppm output in MPI-IO, (started) and output in parallel hdf5, netcdf

```
$ cd parIO/nbody
```

Write parallel hdf5, netcdf, MPI-IO outputs for gravitational particles (FORTRAN)

Conventions for HDF5

- XDMF
- An XML description of your HDF5 files
- A way of encoding "conventions" for HDF5
- Important for interoperatbility (eg, w/ viz packages)



Adaptable IO System

- ADIOS
- A library for IO for scientific code
- Uses MPIIO, HDF5, etc... under the hood
- Allows changing of IO strategy, method; no rewriting code and maybe not even a recompile.

parIO/adios/parallel2darray.{c,f90}

```
void writeadiosfile(rundata_t *rundata, double **dens, double ***vel) {
    int          adios_err=0;
    uint64_t     adios_groupsize, adios_totalsize;
    int64_t      adios_handle;
    MPI_Comm     comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename, "w", &comm);
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

parIO/adios/{,f}array_global.xml

```
<?xml version="1.0"?>
<adios-config host-language="C">

    <adios-group name="ArrayData" coordination-communicator="comm">
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundata->globalny"
                       offsets="0,rundata->startx,rundata->starty">
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata->localny" />
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata->globalny"
                       offsets="rundata->startx,rundata->starty">
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->localny" />
        </global-bounds>
    </adios-group>

<method group="ArrayData" method="PHDF5" />

<buffer size-MB="2" allocate-time="now"/>

</adios-config>
```

ADIOS workflow

- Write XML file describing data, layout
- gpp.py [file].xml - generates C or Fortran code: adios calls, size calculation
- Build code
- Separates data layout, code.

```
<?xml version="1.0"?>
<adios-config host-language="C">
    <adios-group name="ArrayData" coordination-communicator="
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundat
                       offsets="0,rundata->startx,rundata->st
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata-
                       offsets="rundata->startx,rundata->star
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->
        </global-bounds>
    </adios-group>
<method group="ArrayData" method="PHDF5" />
<buffer size-MB="2" allocate-time="now"/>
</adios-config>
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double
    int         adios_err=0;
    uint64_t    adios_groupsize, adios_totalsize;
    int64_t     adios_handle;
    MPI_Comm    comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

ADIOS workflow

- Separation isn't perfect; xml file references code variables, etc.
- But allows "componentization" of I/O.
- Changes that don't result in changes to grwrite_Array.ch don't require recompilation (eg, only changing number, size of variables in group).

```
<?xml version="1.0"?>
<adios-config host-language="C">
    <adios-group name="ArrayData" coordination-communicator="
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundat
                       offsets="0,rundata->startx,rundata->st
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata-
                       offsets="rundata->startx,rundata->star
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->
        </global-bounds>
    </adios-group>
<method group="ArrayData" method="PHDF5" />
<buffer size-MB="2" allocate-time="now"/>
</adios-config>
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double
    int         adios_err=0;
    uint64_t    adios_groupsize, adios_totalsize;
    int64_t     adios_handle;
    MPI_Comm    comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

Variable Groups

- Multiple groups of variables possible: (eg) restart files vs. files for analysis
- Variables can appear in mutiple groups
- Each group can be handled with different methods

```
<?xml version="1.0"?>
<adios-config host-language="C">
    <adios-group name="ArrayData" coordination-communicator="
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundat
                       offsets="0,rundata->startx,rundata->st
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata-
                       offsets="rundata->startx,rundata->star
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->
        </global-bounds>
    </adios-group>
<method group="ArrayData" method="PHDF5" />
<buffer size-MB="2" allocate-time="now"/>
</adios-config>
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double
    int         adios_err=0;
    uint64_t    adios_groupsize, adios_totalsize;
    int64_t     adios_handle;
    MPI_Comm    comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

I/O methods

- Possible methods: parallel HDF5 (PHDF5), NetCDF (NC4), one-per-process posix files (POSIX), it's own native format (BP) using MPI-IO (MPI)
- Change between methods: edit xml file, that's it.
- P-1 (PHDF5, NC4,MPI), P-P (POSIX), or even P-M possible (PHDF5, etc with multiple communicators)

```
<?xml version="1.0"?>
<adios-config host-language="C">
    <adios-group name="ArrayData" coordination-communicator="
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundat
                       offsets="0,rundata->startx,rundata->st
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata-
                       offsets="rundata->startx,rundata->star
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->
        </global-bounds>
    </adios-group>
<method group="ArrayData" method="PHDF5" />
<buffer size-MB="2" allocate-time="now"/>
</adios-config>
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double
    int         adios_err=0;
    uint64_t    adios_groupsize, adios_totalsize;
    int64_t     adios_handle;
    MPI_Comm    comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

Simplifies IO code

- Even if you aren't planning to switch between IO strategies, can greatly simplify code
- Many mechanical steps (eg, pasting together rectangular multi-dimentional arrays) done for you.
- Eliminates tedious, error-prone boilerplate code

```
<?xml version="1.0"?>
<adios-config host-language="C">
    <adios-group name="ArrayData" coordination-communicator="
        <var name="rundata->localnx"  type="integer" />
        <var name="rundata->localny"  type="integer" />
        <var name="rundata->globalnx" type="integer" />
        <var name="rundata->globalny" type="integer" />
        <var name="rundata->startx"   type="integer" />
        <var name="rundata->starty"   type="integer" />
        <var name="size" type="integer" />
        <global-bounds dimensions="2,rundata->globalnx,rundat
                       offsets="0,rundata->startx,rundata->st
           <var name="vel" gwrite="vel[0][0]" type="double"
                       dimensions="2,rundata->localnx,rundata
        </global-bounds>
        <global-bounds dimensions="rundata->globalnx,rundata-
                       offsets="rundata->startx,rundata->star
           <var name="dens" gwrite="dens[0]" type="double"
                       dimensions="rundata->localnx,rundata->
        </global-bounds>
    </adios-group>
<method group="ArrayData" method="PHDF5" />
<buffer size-MB="2" allocate-time="now"/>
</adios-config>
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double
    int          adios_err=0;
    uint64_t     adios_groupsize, adios_totalsize;
    int64_t      adios_handle;
    MPI_Comm     comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

```
void writeadiosfile(rundata_t *rundata, double **dens, double ***vel) {
    int           adios_err=0;
    uint64_t      adios_groupsize, adios_totalsize;
    int64_t       adios_handle;
    MPI_Comm      comm = MPI_COMM_WORLD;
    int size;

    MPI_Comm_size(comm, &size);

    adios_init ("adios_global.xml");
    adios_open (&adios_handle, "ArrayData", rundata->filename, "w", &comm);
    #include "gwrite_ArrayData.ch"

    if (adios_err)
        fprintf(stderr,"Error doing adios write.\n");

    adios_close (adios_handle);
}
```

```
void writehdf5file(rundata_t rundata, double **dens, double ***vel) {
    /* identifiers */
    hid_t file_id, arr_group_id, dens_dataset_id, vel_dataset_id;
    hid_t dens_dataspace_id, vel_dataspace_id;
    hid_t loc_dens_dataspace_id, loc_vel_dataspace_id;
    hid_t globaldensspace,globalvelspace;
    hid_t dist_id;
    hid_t fap_id;

    /* sizes */
    hsize_t densdims[2], veldims[3];
    hsize_t locdensdims[2], locveldims[3];

    /* status */
    herr_t status;

    /* MPI-IO hints for performance */
    MPI_Info info;

    /* parameters of the hyperslab */
    hsize_t counts[3];
    hsize_t strides[3];
    hsize_t offsets[3];
    hsize_t blocks[3];
```

1/7

```
/* set the MPI-IO hints for better performance on GPFS */
MPI_Info_create(&info);
MPI_Info_set(info,"IBM_largeblock_io","true");

/* Set up the parallel environment for file access*/
fap_id = H5Pcreate(H5P_FILE_ACCESS);
/* Include the file access property with IBM hint */
H5Pset_fapl_mpio(fap_id, MPI_COMM_WORLD, info);

/* Set up the parallel environment */
dist_id = H5Pcreate(H5P_DATASET_XFER);
/* we'll be writing collectively */
H5Pset_dxpl_mpio(dist_id, H5FD_MPIO_COLLECTIVE);

/* Create a new file - truncate anything existing, use default properties */
file_id = H5Fcreate(rundata.filename, H5F_ACC_TRUNC, H5P_DEFAULT, fap_id);

/* HDF5 routines generally return a negative number on failure.
 * Should check return values! */
if (file_id < 0) {
    fprintf(stderr,"Could not open file %s\n", rundata.filename);
    return;
}
```

2/7

```
/* Create a new group within the new file */
arr_group_id = H5Gcreate(file_id,"/ArrayData", H5P_DEFAULT, H5P_DEFAULT,
                         H5P_DEFAULT);

/* Give this group an attribute listing the time of calculation */
{
    hid_t attr_id,attr_sp_id;
    struct tm *t;
    time_t now;
    int yyyymm;
    now = time(NULL);
    t = localtime(&now);
    yyyymm = (1900+t->tm_year)*100+t->tm_mon;

    attr_sp_id = H5Screate(H5S_SCALAR);
    attr_id = H5Acreate(arr_group_id, "Calculated on (YYYYMM)", H5T_STD_U32LE,
                        attr_sp_id, H5P_DEFAULT, H5P_DEFAULT);
    printf("yymm = %d\n",yyyymm);
    H5Awrite(attr_id, H5T_NATIVE_INT, &yyyymm);
    H5Aclose(attr_id);
    H5Sclose(attr_sp_id);
}

/* Create the data space for the two global datasets. */
densdims[0] = rundata.globalnx; densdims[1] = rundata.globalny;
veldims[0] = 2; veldims[1] = rundata.globalnx; veldims[2] = rundata.globalny;
```

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```
dens_dataspace_id = H5Screate_simple(2, densdims, NULL);
vel_dataspace_id  = H5Screate_simple(3, veldims,  NULL);

/* Create the datasets within the file.
 * H5T_IEEE_F64LE is a standard (IEEE) double precision (64 bit) floating (F) data
 * and will work on any machine.  H5T_NATIVE_DOUBLE would work too, but would give
 * different results on GPC and TCS */

dens_dataset_id = H5Dcreate(file_id, "/ArrayData/dens", H5T_IEEE_F64LE,
                            dens_dataspace_id, H5P_DEFAULT, H5P_DEFAULT, H5P_DEFAUI
vel_dataset_id  = H5Dcreate(file_id, "/ArrayData/vel",  H5T_IEEE_F64LE,
                            vel_dataspace_id,  H5P_DEFAULT, H5P_DEFAULT, H5P_DEFAUI

/* Now create the data space for our sub-regions.   These are the data spaces
 * of our actual local data in memory. */
locdensdims[0] = rundata.localnx; locdensdims[1] = rundata.localny;
locveldims[0] = 2; locveldims[1] = rundata.localnx; locveldims[2] = rundata.localny

loc_dens_dataspace_id = H5Screate_simple(2, locdensdims, NULL);
loc_vel_dataspace_id  = H5Screate_simple(3, locveldims,  NULL);
```

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```
/*
  *
  * Now we have to figure out the `hyperslab' within the global
  * data that corresponds to our local data.
  *
  * Hyperslabs are described by an array of counts, strides, offsets,
  * and block sizes.
  *
  *       |-offx--|
  *       +-------|----|-------+   -+-
  *       |                    |    |
  *       |                    |   offy
  *       |                    |    |
  *       -       +----+       -   -+-
  *       |       |    |       |    |
  *       |       |    |       |  localny
  *       |       |    |       |    |
  *       -       +----+       -   -+-
  *       |                    |
  *       |                    |
  *       +-------|----|-------+
  *               localnx
  *
  *  In this case the blocksizes are (localnx,localny) and the offsets are
  *  (offx,offy) = ((myx)/nxp*globalnx, (myy/nyp)*globalny)
  */
```

```
offsets[0] = (rundata.globalnx/rundata.npx)*rundata.myx;
offsets[1] = (rundata.globalny/rundata.npy)*rundata.myy;
blocks[0]  = rundata.localnx;
blocks[1]  = rundata.localny;
strides[0] = strides[1] = 1;
counts[0] = counts[1] = 1;

/* select this subset of the density variable's space in the file */
globaldensspace = H5Dget_space(dens_dataset_id);
H5Sselect_hyperslab(globaldensspace,H5S_SELECT_SET, offsets, strides, counts, block

/* For the velocities, it's the same thing but there's a count of two,
 * (one for each velocity component) */

offsets[1] = (rundata.globalnx/rundata.npx)*rundata.myx;
offsets[2] = (rundata.globalny/rundata.npy)*rundata.myy;
blocks[1]  = rundata.localnx;
blocks[2]  = rundata.localny;
strides[0] = strides[1] = strides[2] = 1;
counts[0] = 2; counts[1] = counts[2] = 1;
offsets[0] = 0;
blocks[0] = 1;
```

```
    globalvelspace = H5Dget_space(vel_dataset_id);
    H5Sselect_hyperslab(globalvelspace,H5S_SELECT_SET, offsets, strides, counts, blocks

    /* Write the data.  We're writing it from memory, where it is saved
     * in NATIVE_DOUBLE format */
    status = H5Dwrite(dens_dataset_id, H5T_NATIVE_DOUBLE, loc_dens_dataspace_id, global
dist_id, &(dens[0][0]));
    status = H5Dwrite(vel_dataset_id,  H5T_NATIVE_DOUBLE, loc_vel_dataspace_id, globalv
dist_id, &(vel[0][0][0]));

    /* End access to groups & data sets and release resources used by them */
    status = H5Sclose(dens_dataspace_id);
    status = H5Dclose(dens_dataset_id);
    status = H5Sclose(vel_dataspace_id);
    status = H5Dclose(vel_dataset_id);
    status = H5Gclose(arr_group_id);
    status = H5Pclose(fap_id);
    status = H5Pclose(dist_id);

    /* Close the file */
    status = H5Fclose(file_id);
    return;
```

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ADIOS hands-on:

- Modify XML file, try outputting with method of MPI (use bpls or bp2hdf on resulting file), POSIX (Netcdf won't work at this point)
- Try a different IO strategy; do contiguous parallel IO by having single file but with each process' data contiguous in file, one after another. With large file size (--nx=10000 --ny=10000) and 8/16 processes, what are the timings between "straight" PHDF5, MPI, POSIX, and this approach? (And how long would it have taken you to do this without ADIOS?)
- Advanced: Break up MPI_COMM_WORLD into 2 communicators using MPI_Comm_split, call the new communicator comm, and output 2 files from the 8/16 processes using PHDF5 or MPI.