NetCDF for Developers and Data Providers

Russ Rew, UCAR Unidata

ICTP Advanced School on High Performance and Grid Computing

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Overview

- Background and motivation
- What is netCDF?
- Data models
- Utilities: ncdump, ncgen, nccopy
- Exercises
- Application Programming Interfaces (API's)
- Remote access and OPeNDAP
- Chunking and compression
- Parallel I/O

Application Programming Interfaces (API's)

Programming interfaces to netCDF data

All netCDF APIs are currently implemented over either the C or Java library.

- NetCDF C interface was first API, developed in 1988
- Fortran-77 interface added as a thin layer over C library
- Interfaces for Java, Perl, and first C++ library developed at Unidata
- Collaborated on a Fortran-90 interface
- Other contributed C-based interfaces include Python, Perl, Ruby, NCL, Matlab, IDL, R, Objective C, Ada, and new C++ API for netCDF-4
- Java is most advanced netCDF API, best for use on servers

The C API

- Core library on which all non-Java APIs are built
- Strengths:
  - Well-documented: C Users Guide, man pages for reference
  - Comprehensively tested when library built from source
  - Good support: answers for many questions available
  - Many users: one of the most widely used netCDF interfaces.
  - Type-safe interfaces avoid “void *” arguments and catch compile-time errors
  - The **ncgen** utility can generate C code from CDL

C example for reading data

```c
#include <netcdf.h>
   ...
/* Handle errors by printing an error message and exiting */
#define ERR(e) {printf("Error: %s\n", nc_strerror(e)); exit(ERRCODE);}
   ...
   /* netCDF file ID and variable ID */
   int ncid, varid;
   /* array into which we will read values of 2D netCDF variable */
   double rh_array[NLAT][NLON];
   ...
   /* Open file with read-only access, indicated by NC_NOWRITE flag */
   if ((retval = nc_open("foo.nc", NC_NOWRITE, &ncid)))
        ERR(retval);
   /* Get the id of the variable named "rh" */
   if ((retval = nc_inq_varid(ncid, "rh", &varid)))
        ERR(retval);
   /* Read variable "rh" as doubles, rh_array must be big enough! */
   if ((retval = nc_get_var_double(ncid, varid, &rh_array[0][0])))
        ERR(retval);
   /* Close the file, freeing all resources. */
   if ((retval = nc_close(ncid)))
        ERR(retval);
```

The Fortran-90 API

Provides current Fortran support for modelers and scientists

- Strengths:
  - Well-documented: Fortran-90 Users Guide, man pages for reference
  - Overloads var_put and var_get functions for all types and shapes
  - Optional arguments simplify API
  - Many users: one of the most widely used netCDF interfaces
- Other characteristics
  - Currently implemented in Fortran-90 as thin layer on Fortran-77 library
  - No **ncgen** utility support (yet) for generating F90 code from CDL

Fortran-90 API example for reading data

```
use netcdf
   ...
! check(status) function prints error message and exits
  ...
! netCDF ID for the file and data variable
  integer :: ncid, varid
! array into which we will read values of 2D netCDF variable
  double rh_array[NLON][NLAT]   ! reversed index order from CDL
  ...
! Open file with read-only access, indicated by NF90_NOWRITE flag
  call check( nf90_open("foo.nc", NF90_NOWRITE, ncid) )

! Get the id of the variable named "rh"
  call check( nf90_inq_varid(ncid, "rh", varid) )

! Read whole variable "rh" as double, rh_array must be big enough!
  call check( nf90_get_var(ncid, varid, rh_array) )
  ...
! Close the file, freeing all resources.
  call check( nf90_close(ncid) )
```

Language independence

- The netCDF data model and format are language-independent.
  - Data written from any language interface can be read from any other language interface
- Fortran API uses Fortran dimension row-major order, 1-based indexing
- Unlike netCDF, CDL is not quite language neutral

```
variables:
   float rh(time, lat, lon) ;
```

CDL

→

```
! time slice
  real rh(lon, lat) ;
```

Fortran

Equivalent examples from various APIs

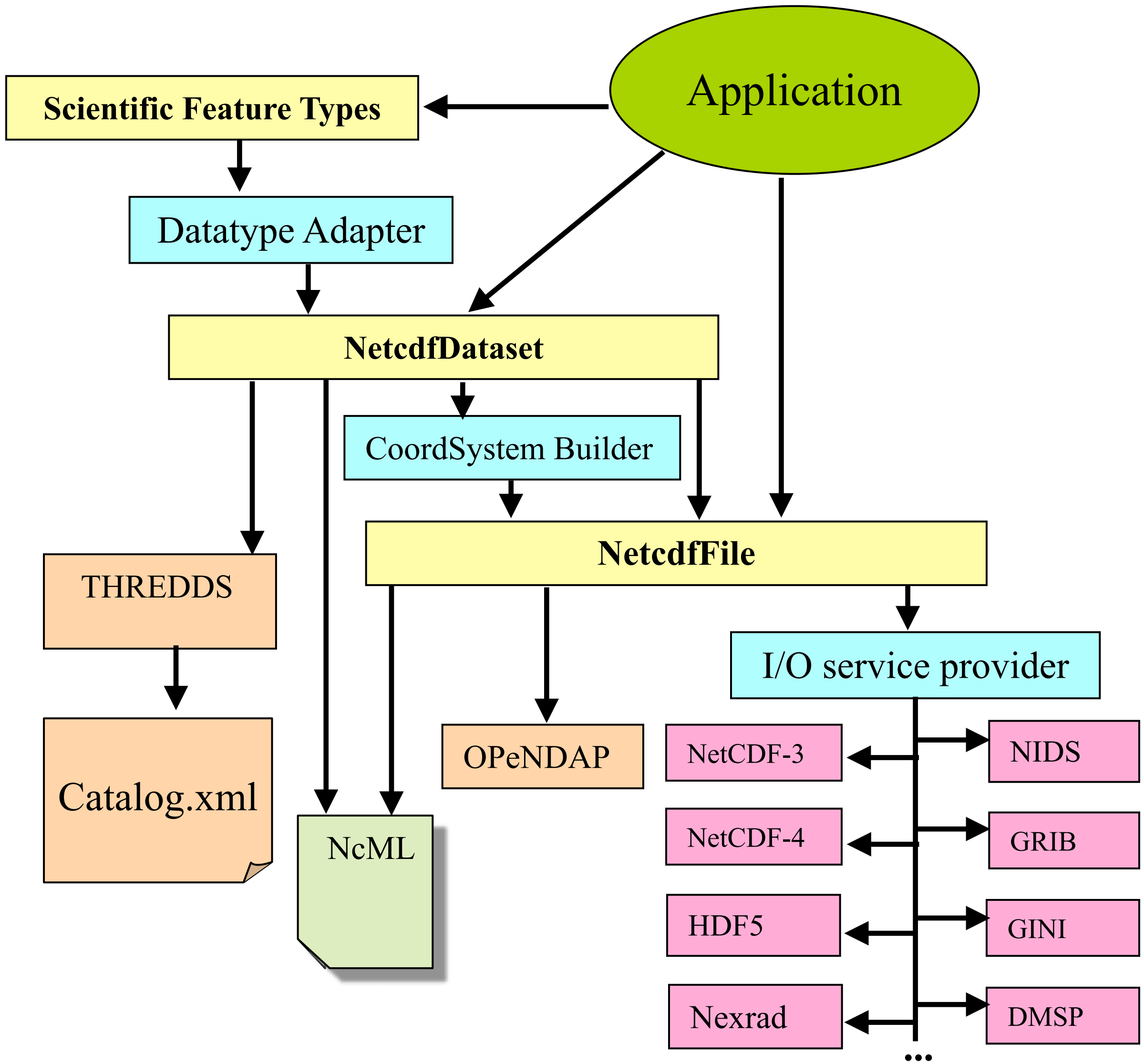
- Examples of complete sample programs for writing and reading netCDF data from various language interfaces are available from the netCDF program examples page http://www.unidata.ucar.edu/netcdf/examples/programs/

Fortran-77 Fortran-90 C

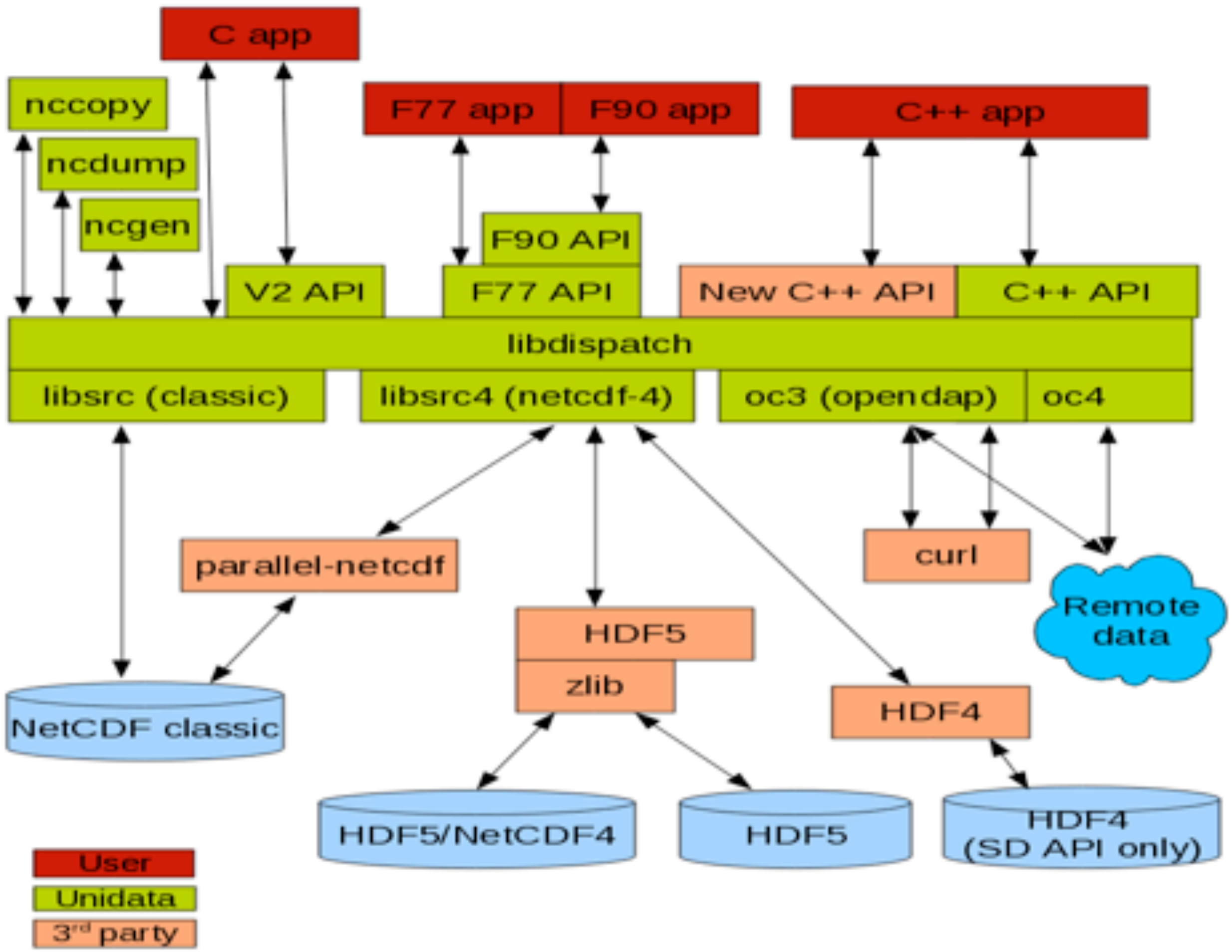
MATLAB IDL C++

Perl python™ JAVA

Java netCDF library architecture



C netCDF library architecture



Remote access and OPeNDAP

Alternatives for remote data access

- Whole file access
  - ftp, scp, sftp, http for "small" (< 10 GB) files
  - tar for directories
  - gridFTP or Globus Online for large files: fast, parallel, requires certificate
- Subset access
  - OPeNDAP (open network data access protocol)
  - Open Geospatial Consortium services: WCS, WMS, WFS, …
  - Database queries

When is subset access important?

- For remote accesses to small parts of large files
  - A few variables out of many
  - A small geographic region from a global dataset
  - A small time range from a long time series
- When visualizing or analyzing data subsets
  - One 2D level of atmosphere or ocean
  - One cross section of multidimensional data
- When files are archived at a granularity too large for use or downloading

What are OPeNDAP and DAP?

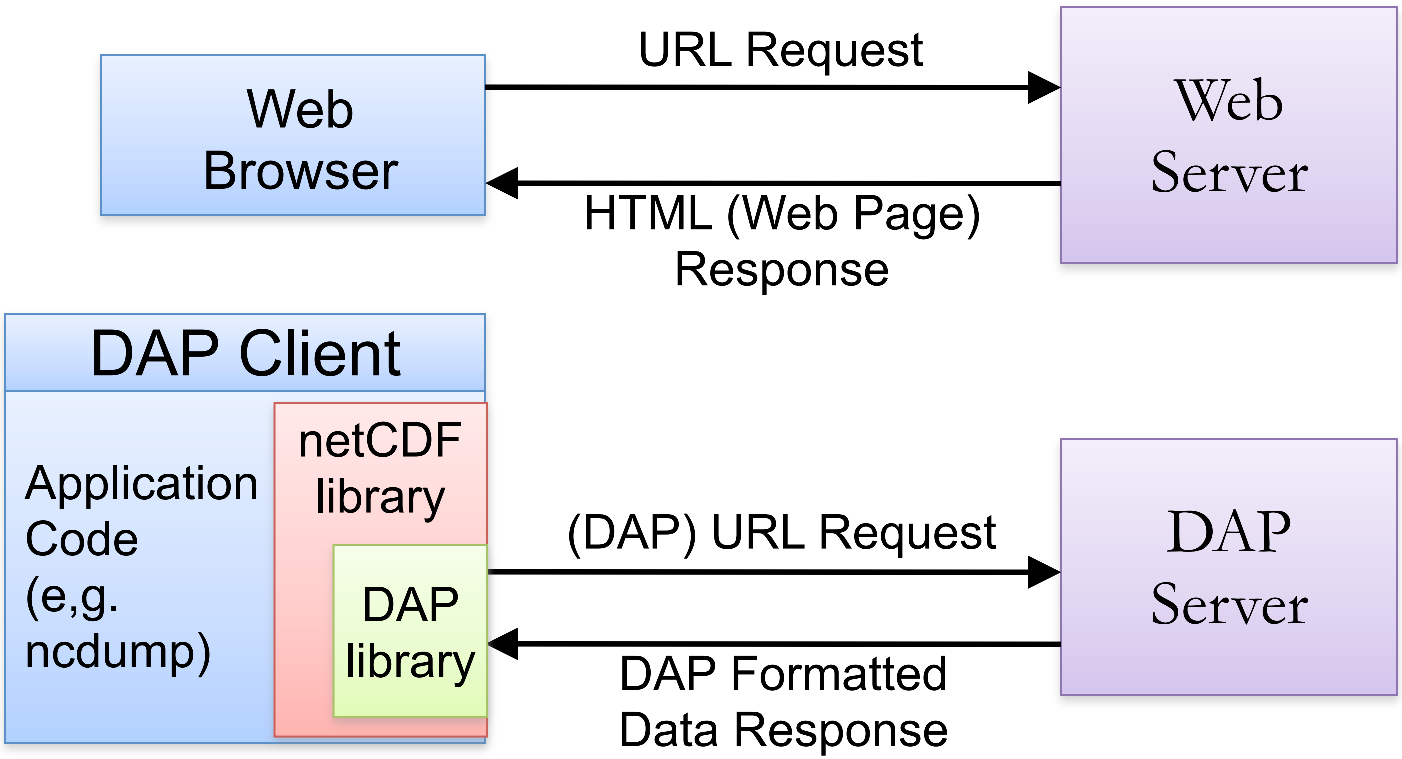
- DAP is a widely supported data access protocol for accessing remote science data over http
- The standard and reference client/server software are maintained by the OPeNDAP organization
  http://www.opendap.org/
- DAP was designed for accessing a wide variety of data sources and formats
- "DAP" and "OPeNDAP" are often used interchangeably

OPeNDAP and netCDF

- Unidata has merged OPeNDAP client access into both Java- and C-based netCDF libraries.
- This supports transparent remote access to DAP Data Servers through the netCDF API.
- Remote access allows any application linked to the netCDF library to retrieve subsets of data stored on DAP servers across the Internet.
- Only the minimal amount of needed data will be accessed
  - DAP can be much faster than whole file access, such as FTP

DAP client-server architecture

- DAP data access is analogous to accessing a web page through a web browser



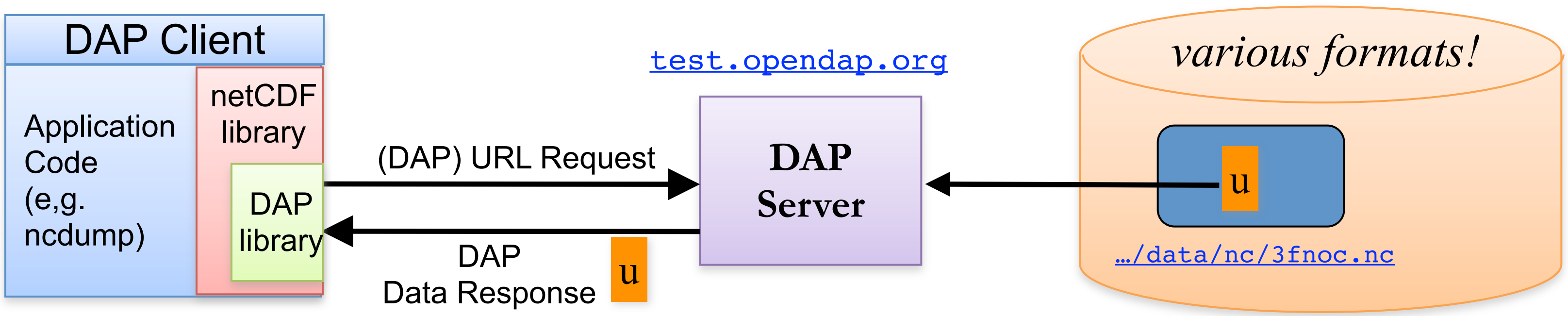
Specifying a DAP data source

- Use a URL that refers to the DAP server containing the data
- Used in place of a file name in application or netCDF API call
- Example for whole file: http://test.opendap.org/opendap/data/nc/3fnoc.nc
- Example for 3 variables out of file

  http://test.opendap.org/opendap/data/nc/3fnoc.nc?lat,lon,time
- Example for subarray of one variable

  http://test.opendap.org/opendap/data/nc/3fnoc.nc?u[2:5][0:4][0:5]
- When used in command-line, URL should usually be quoted:

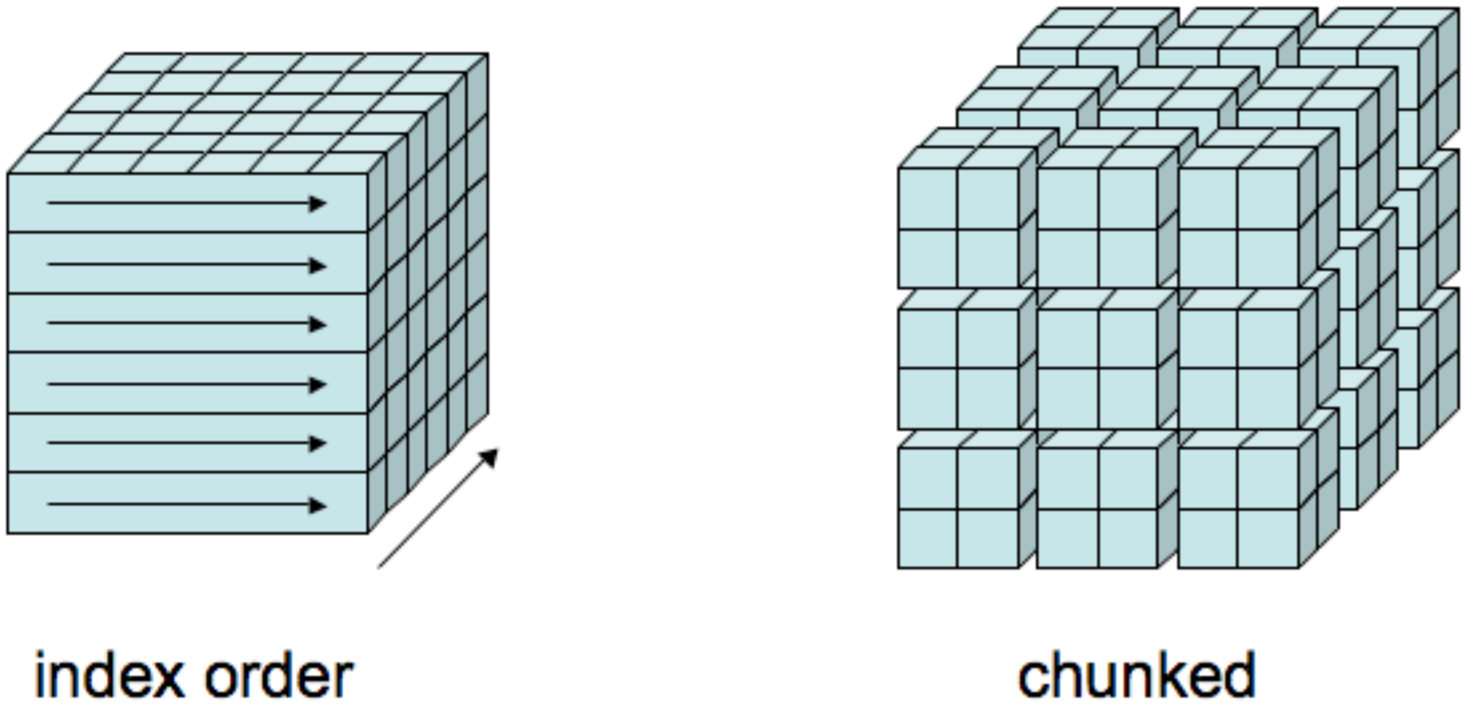
```
ncdump "http://test.opendap.org/opendap/data/nc/3fnoc.nc?u"
```



Chunking and compression

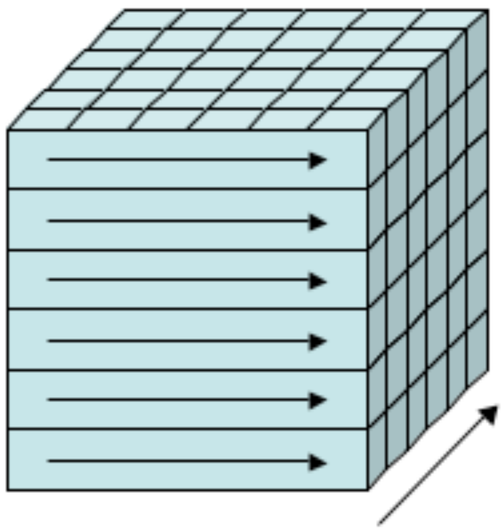
Motivation for chunking

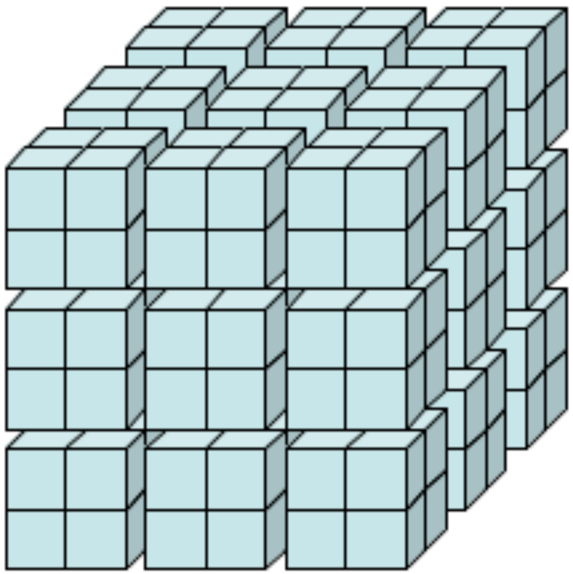
- **Problem**: reading a small amount of data along the wrong direction in a multidimensional variable can be *very* slow:



Motivation for chunking

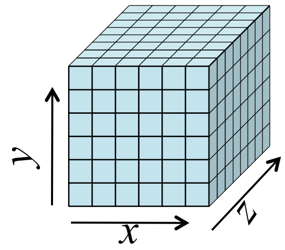
- **Solution**: storing the data in "chunks" along each dimension in a multidimensional variable makes access along any dimension similar



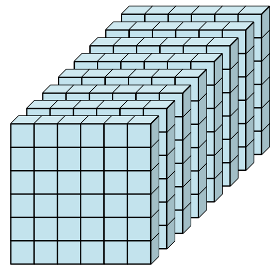


Example: accessing cross-sections

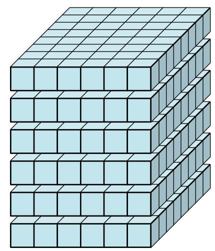
- "Toy" example: accessing a 6 x 6 x 8 array on a system with small disk blocks



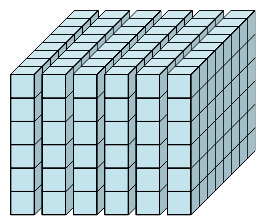
- If array is stored contiguously, then (ignoring caching) number of disk accesses needed to
  - read a single x,y 2D cross-section: 1
  - read a single x,z or y,z 2D cross-section: 8
  - read whole array using x,y slices: 8
  - read whole array using x,z or y,z slices: 48



  - read a single 1D vector along x or y axis: 1
  - read a single 1D vector along z axis: 8
  - read whole array using 1D vectors along x or y axis: 8

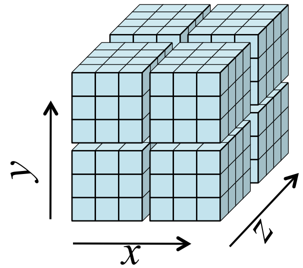


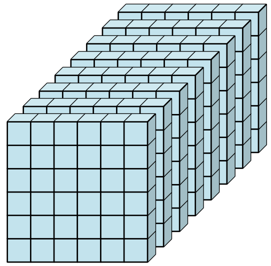
  - read whole array using 1D vectors along z axis: 288
- Contiguous same as 6 x 6 x 1 chunks, try 3 x 3 x 4 chunks …

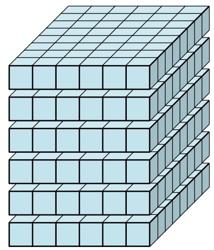


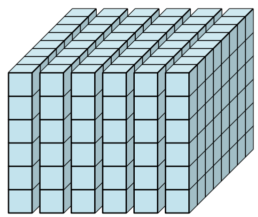
Accessing cross-sections with chunking

- Same data: 6 x 6 x 8 array
- If array is stored using 3 x 3 x 4 chunks, then number of disk accesses needed to
  - read a single x,y 2D cross-section: 4
  - read a single x,z or y,z 2D cross-section: 4
  - read whole array using x,y slices: 32
  - read whole array using x,z or y,z slices: 32
  - read a single 1D vector along x or y axis: 2
  - read a single 1D vector along z axis: 2
  - read whole array using 1D vectors on x or y axis: 96
  - read whole array using 1D vectors along z axis: 72





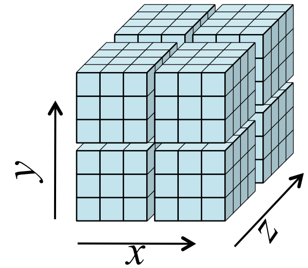


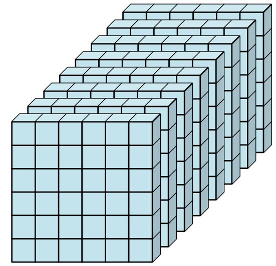


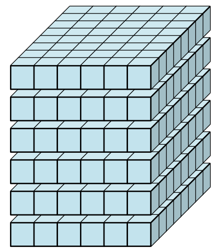
Accessing cross-sections with chunking

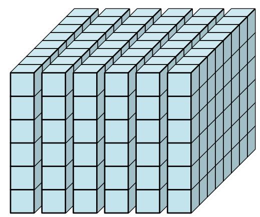
- Same data: 6 x 6 x 8 array

Access	Contiguous (disk accesses)	Chunking (disk accesses)
2D x,y cross-section	1	4
2D x,z or y,z cross-section	8	4
3D array using x,y slices	8	32
3D array using x,z or y,z slices	48	32
1D vector along x or y axis	1	2
1D vector along z axis	8	2
3D array using x or y vectors	8	96
3D array using z vectors	288	72



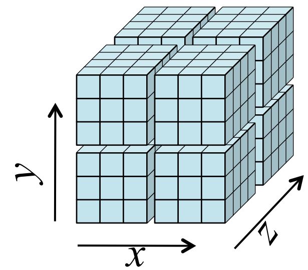


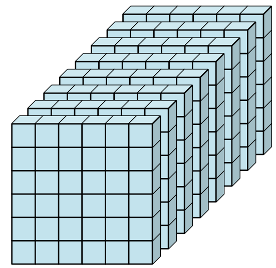


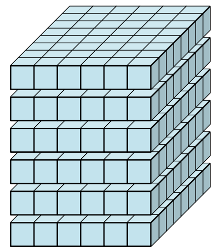


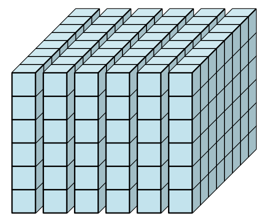
Actual timings accessing cross-sections with chunking

- 432 x 432 x 432 array of floats with chunk sizes of 36 x 36 x 36









Access	Contiguous (seconds)	Chunking (seconds)	Slowdown or speedup
2D x,y cross-section write	0.559	1.97	3.5 x slower
2D x,z cross-section write	18.1	1.5	12 x faster
2D y,z cross-section write	223	9.55	23 x faster
2D x,y cross-section read	0.353	1.06	3 x slower
2D x,z cross-section read	6.22	1.45	4.3 x faster
2D y,z cross-section read	77.1	7.68	10 x faster

- Fast accesses slow down a little, slow accesses speed up a lot

Benefits of chunking

- As a general principle, organize data for readers, not writer
  - Chunking should match most common access patterns
  - Chunking may also improve compression
- Chunked storage can provide significant performance benefits
  - Allows efficient access to multidimensional data along multiple axes
  - Default chunking parameters make access performance similar along different dimensions
  - In netCDF-4 (with HDF5 storage) variables may be chunked independently with custom chunk sizes
  - Can improve I/O performance for large arrays and compressed variables

Compression: why not just use zip?

- Unix utilities are available for compressing whole files, e.g. bzip2, gzip, zip, compress. Why not just use one of those?
  - Accessing data from a compressed file requires uncompressing whole file first
  - So accessing a small amount of data from a large compressed file can be very slow
  - Changing one value in a compressed file requires uncompressing it, writing the new value, and recompressing it
- ***Solution***: chunking and per-variable compression

Compression in netCDF-4

- Readers access data from compressed variables transparently, without needing to know they are compressed
- Compressed variables are stored with chunked storage
- Each chunk is compressed or uncompressed independently
- Permits efficient access to small subsets of a large compressed variable without uncompressing entire variable
- Per-variable chunk caches keep recently accessed chunks uncompressed
- Better compression can be achieved with custom chunking.
  - example: horizontal layers of the atmosphere for a variable that is fairly uniform within a layer, such as temperature
  - Per-variable compression means variables may be compressed independently

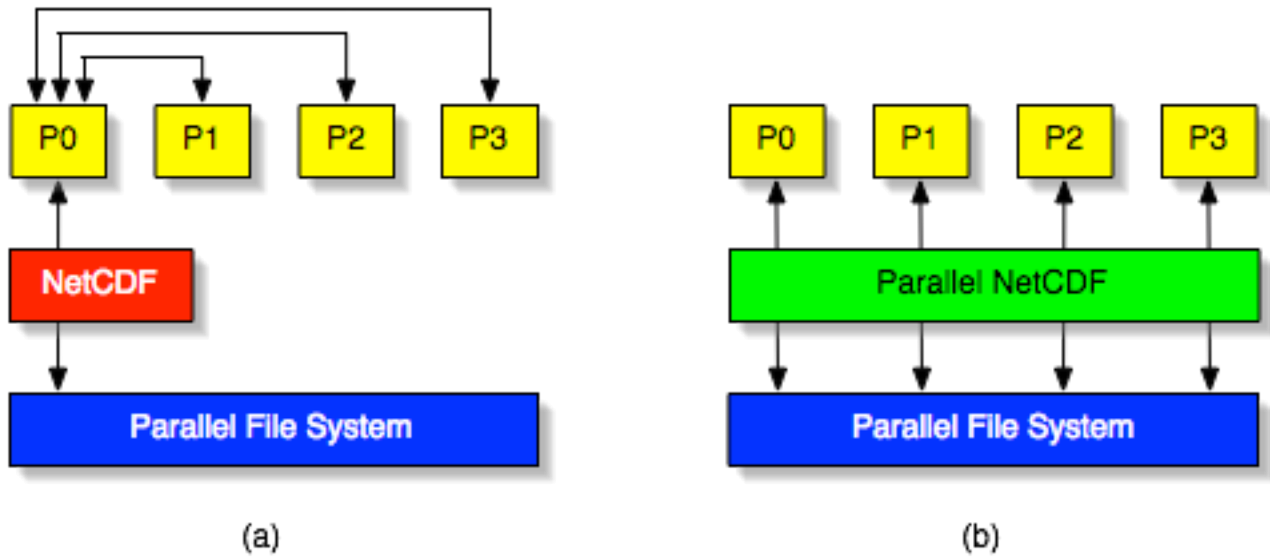
Benefits of netCDF-4 classic model format

- What is the netCDF-4 classic model format?
  - Uses classic data model for simplicity, compatibility
  - Uses netCDF-4 (HDF5-based) storage for performance features
- This format has become popular for several reasons:
  - Easy to use: specify format only in netCDF create call
  - Features like chunking, compression available to writers
  - Data written in this format can be read transparently by old programs, after relinking to new library
- Supports easier transition from netCDF-3

Parallel I/O

Why parallel I/O?

- Gets around some input/output bottlenecks in multi-processor systems
- Lets each processor read and write data independently



What is parallel I/O?

- A parallel I/O file system is required for much improvement in I/O throughput
- NetCDF-4 works with the Message Passing Interface, version 2 (MPI2)
- Any supercomputer will have an MPI2 library
- For netCDF testing we use the MPICH2 library

The Argonne parallel-netCDF package

- parallel-netcdf (formerly "pnetcdf") from Argonne Labs and Northwestern University can be used for parallel I/O with classic netCDF data.
- Not Unidata software, but well-tested and maintained
- Uses MPI I/O to perform parallel I/O, a complete rewrite of the core C library using MPI I/O
- Implements different API from netCDF, making portability with other netCDF code a problem
- However, netCDF-4 can now use the parallel netCDF library for classic and 64-bit offset files using parallel I/O
- Use the NC_PNETCDF flag (or NF90_PNETCDF for Fortran):

```
if (nc_create_par(file_name, NC_PNETCDF, mpicomm, info, &ncid))
    ERR;
```

Parallel I/O in netCDF-4

- Provides the parallel I/O features of HDF5 with a netCDF API
- Allows *n* processes on *m* processors to read and write netCDF data, where *n* and *m* are integers usually < 10K
- Requires a library implementing MPI2, for example MPICH2
- HDF5 must be built with --enable-parallel
- Typically CC environment variable is set to mpicc, and FC to mpifc . You must build HDF5 and netCDF-4 with same compiler and compiler options.
- The netCDF configure script will detect the parallel capability of HDF5 and build the netCDF-4 parallel I/O features automatically.
- For parallel applications you must include "netcdf_par.h" before netcdf.h.
- Parallel tests output can tell you a lot about your parallel platform.

Using parallel I/O in netCDF-4

- Special nc_create_par and nc_open_par functions are used to create/open a netCDF file.
- The files they open are normal NetCDF-4/HDF5 files, but these functions also take MPI parameters.
- Parallel access is not a characteristic of data file, but the way it was opened.

```
external int
nc_create_par(const char *path, int cmode,
       MPI_Comm comm, MPI_Info info, int *ncidp);

external int
nc_open_par(const char *path, int mode,
       MPI_Comm comm, MPI_Info info, int *ncidp);
```

Collective and independent operations

- Some netCDF operations are ***collective*** (must be done by all processes at the same time)
- Others are ***independent*** (can be done by any process at any time)
- All netCDF metadata writing operations are collective. That is, all creation of groups, types, variables, dimensions, or attributes.
- Data reads and writes may be independent (the default) or collective.
- To make writes to a variable collective, call the

```
if( nc_var_par_access(ncid, varid, NC_COLLECTIVE) )
   ERR;
```

Conclusion

- Data providers may begin to use compression/chunking with confidence that most users and software can read it transparently, after relinking with netCDF-4
- Developers may adapt software to netCDF-4 format by relinking
- Developers may adapt software to enhanced data model incrementally, with examples that such adaptation is practical
- Upgrading software to make use of higher-level abstractions of netCDF-4 enhanced data model has significant benefits
  - Data providers can use more natural representation of complex data semantics
  - More natural conventions become possible
  - End users can access other types of data through netCDF APIs
- As we keep pushing common tasks into libraries, scientists can focus on doing science instead of data management

Thank you!