# Introduction to netCDF formats, data models, and utilities

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#### Introduction to netCDF

#### Covered

- Overview
- Formats
- Data models
- Utilities
- Exercises

#### Not covered

- Building and installing
- Library architecture
- Application programming interfaces for C, Java, ...
- Remote access with DAP
- CF conventions
- Compression and chunking
- Diskless files
- Parallel I/O, HPC issues
- Future plans

See most recent netCDF workshop for subjects on right





# Overview of netCDF





# History of netCDF development

Knowing how netCDF evolved explains some of the oddities of its architecture.



1988: NetCDF developed at Unidata



1996: NetCDF v3.0 new API



2008: NetCDF v4.0 uses HDF5



2012: NetCDF 4.2.1 Windows® support, "diskless I/O"





2004: NetCDF v3.6 64-bit offset format



2011: NetCDF v4.1 OPeNDAP client, HDF4. pnetcdf







# More than just a file format ...





# More than just a file format ...







# More than just a file format ...



At its simplest, it's also:

- A data model
- An application programming interface (API)
- Software implementing the API

Together, the format, data model, API, and software support the creation, access, and sharing of scientific data.





# What is netCDF, really?

- Four format variants
  - Classic format and 64-bit offset format for netCDF-3
  - NetCDF-4 format and netCDF-4 classic model format
- Two data models
  - Classic model (for netCDF-3)
  - Enhanced model (for netCDF-4)
- Many language APIs
  - C-based (Python, C, Fortran, C++, R, Ruby, ...)
  - Java-based (Java, MATLAB, ...)
- Unidata and 3<sup>rd</sup>-party software (NCO, NCL, CDO, ...)

Do users have to know about these complications? Not usually, thanks to ...





#### Version compatibility and transparency

You mostly don't need to be aware of version complications, because **new** versions of Unidata netCDF software continue to support

- All previous netCDF formats and their variants
- All previous netCDF data models
- All previous APIs\*

\*Disclaimer: exceptions for bugs, early releases, documented experiments

Also, netCDF data written with any language API is readable through other language APIs. \*

\*Exception: currently some advanced netCDF-4 features are only available from C and Fortran APIs







To ensure future access to existing data archives, Unidata is committed to compatibility of:

- Data access: new versions of netCDF software will provide read and write access to previously stored netCDF data.
- Programming interfaces: C and Fortran programs using documented netCDF interfaces from previous versions will work without change\* with new versions of netCDF software.
- **Future versions**: Unidata will continue to support both data access compatibility and program compatibility in future netCDF releases\*.

\*See reverse side of this slide for disclaimers and exceptions.

# Summary: netCDF formats, data models, APIs

- File formats for portable data and metadata
  - Support array-oriented scientific data and metadata
  - Make data self-describing, portable, scalable, remotely accessible, archivable, and structured
- Data models for geosciences
  - o Classic: simplest model -- dimensions, variables, and attributes
  - Enhanced: more complex and powerful model adds groups and user-defined types
- APIs for building applications and services
  - o Unidata supports and maintains C and Java implementations.
  - Unidata provides best-effort support for Fortran and C++ implementations.
  - Open source community and 3<sup>rd</sup> parties support and maintain other APIs, including netcdf4-python for Python.





# netCDF formats





#### Characteristics of netCDF formats 1

#### NetCDF data is:

- **Self-describing:** You can include metadata as well as data, name variables, locate data in time and space, store units of measure, conform to metadata standards.
- **Portable:** You can write on one platform and read it on other platforms.
- **Scalable:** You can access small subsets of large datasets efficiently.
- **Appendable:** You can add new data efficiently without copying existing data. You can add new metadata without changing existing programs.





#### Characteristics of netCDF formats 2

- Remotely accessible: You can access data in netCDF and other formats from remote servers using OPeNDAP protocols.
- Archivable: You can access earlier versions of netCDF formats using current and future versions of software.
- Structured: You can use a variety of types and data structures to capture the meaning in your data.





#### **NetCDF** classic format

#### Strengths

- ✓ Simple to understand and explain
- ✓ Supported by many applications
- ✓ Standardized for used in many archives, data projects
- Mature conventions and best practices available

#### Limitations

- No support for efficient compression
- Schema changes slowed by copying data
- 4 GiB limits on variable sizes
- Performance issues reading data in different order than written





#### NetCDF-4 format

#### Strengths

- ✓ Efficient compression from HDF5 storage
- ✓ Efficient access with HDF5 chunking
- ✓ Efficient schema changes supported
- ✓ Variables can be huge
- Good testing and support for high performance computing platforms

#### Limitations

- Zlib compression sometimes not competitive
- Chunking defaults often not appropriate, need careful tuning
- Complex format discourages multiple implementations
- Workarounds required to handle lack of HDF5 support for shared, named dimensions





#### NetCDF-4 classic-model transitional "format"

netCDF-3

- Compatible with existing applications
- Simplest data model and API

netCDF-4 classic model

- Can be accessed through netCDF-3 APIs, compatible with classic data model
- Uses netCDF-4/HDF5 storage for performance: compression, chunking, ...
- Transparent access after library update

netCDF-4

- Requires netCDF-4 APIs to access enhanced model features, such as strings, groups, and user-defined types
- Good for new data and applications





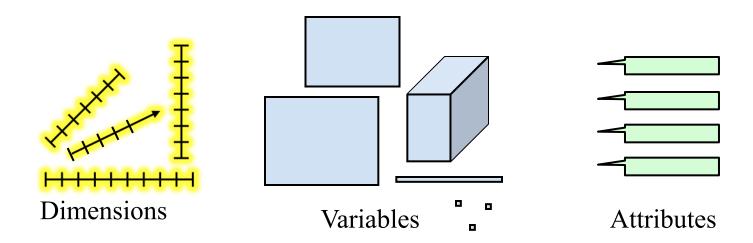
# netCDF data models





#### The netCDF classic data model

- NetCDF data has named dimensions, variables, and attributes.
- *Dimensions* are for specifying shapes of variables
- Variables are for data, attributes are for metadata
- Attributes may apply to a whole dataset or to a variable
- Variables may share dimensions, indicating a common grid.
- One dimension may be of unlimited length.
- Each variable or attribute has a *type*: char, byte, short, int, float, double







#### The netCDF classic data model (UML)

#### NetCDF Data has

Dimensions (lat, lon, level, time, ...)

Variables (temperature, pressure, ...)

Attributes (units, valid\_range, ...)

Each dimension has

Name, length

Each variable has

Name, shape, type, attributes

N-dimensional array of values

Each attribute has

Name, type, value(s)

Variables may share dimensions

Represents shared coordinates, grids

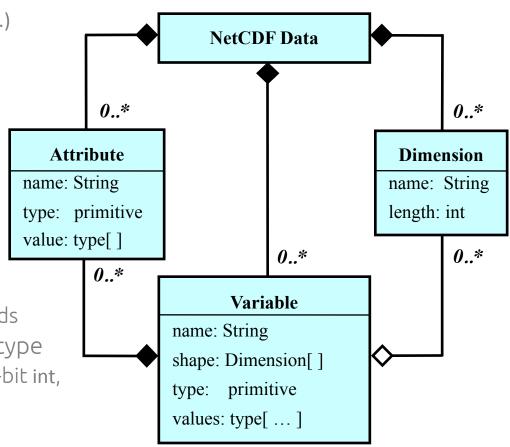
Variable and attribute values are of type

Numeric: 8-bit byte, 16-bit short, 32-bit int,

32-bit float, 64-bit double

Character: arrays of char for text

UML = Unified Modeling Language

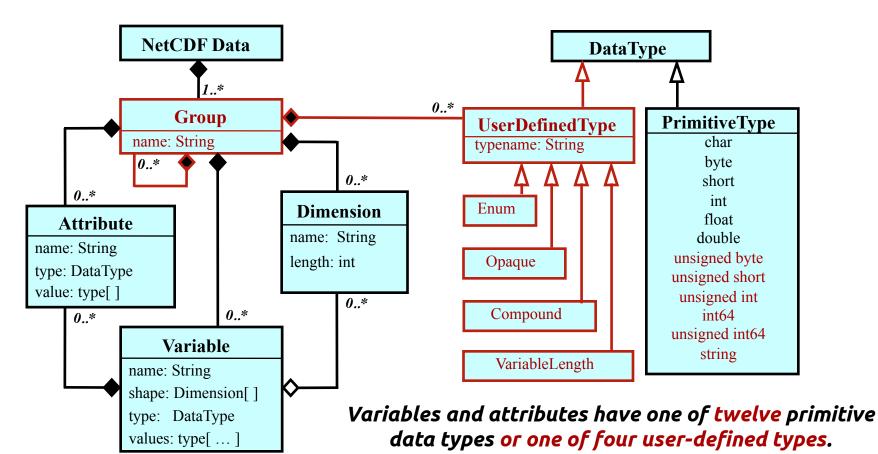






#### The netCDF-4 enhanced data model

A file has a top-level unnamed group. Each group may contain one or more named subgroups, user-defined types, variables, dimensions, and attributes. Variables also have attributes. Variables may share dimensions, indicating a common grid. One or more dimensions may be of unlimited length.







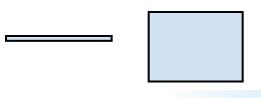
#### Variables or attributes?

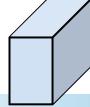
#### **Variables**

- intended for data
- can hold arrays too large for memory
- may be multidimensional
- support partial access (only a subset of values)
- values may be changed, more data may be appended
- may have attributes
- shape specified with netCDF dimensions
- not read until accessed



- intended for metadata
- for small units of information that fit in memory
- for single values, strings, or small
  1-D arrays
- atomic access, must be written or read all at once
- values typically don't change after creation
- an attribute may not have attributes
- read when file opened









#### NetCDF classic data model

#### Strengths

- ✓ Data model simple to understand and explain
- ✓ Can be efficiently implemented
- Representation good for gridded multidimensional data
- ✓ Shared dimensions useful for coordinate systems
- ✓ Generic applications easy to develop

#### Limitations

- Small set of primitive types
- Data model limited to multidimensional arrays, (name, value) pairs
- Flat name space that hinders organizing many data objects
- Lack of nested structures, variable-length types, enumerations





#### NetCDF-4 enhanced data model

#### Strengths

- ✓ Increased representational power for more complex data
- Adds shared, named dimensions to HDF5 data model
- ✓ Compatible with netCDF-3 classic data model
- ✓ Adds useful primitive types
- ✓ Provides nesting: hierarchical groups, recursive data types

#### Limitations

- More complex than classic data model
- Effort required to develop general tools and applications
- Adoption proceeding slowly
- Best practices and conventions still maturing





# netCDF utilities (netCDF without programming)





#### Common Data Language (CDL)

Text notation for netCDF metadata and data

```
netcdf example { // example of CDL notation
 dimensions:
         x = 2;
         y = 8 ;
 variables:
         float rh(x, y);
                rh:units = "percent";
                rh:long name = "relative humidity";
 // global attributes
         :title = "simple example, lacks conventions";
 data:
  rh =
   2, 3, 5, 7, 11, 13, 17, 19,
   23, 29, 31, 37, 41, 43, 47, 53;
}
```

Example with 2 dimensions (x and y), 1 variable (rh), 2 variable attributes (units and long\_name), 1 global attribute (title), and 16 data values.





#### Utility programs for netCDF to/from CDL

\$ ncdump -h co2.nc # converts netCDF to CDL

```
netcdf co2 {
dimensions:
       T = 456;
variables:
       float T(T);
              T:units = "months since 1960-01-01";
       float co2(T);
              co2:long name = "CO2 concentration by volume";
              co2:units = "1.0e-6";
              co2: FillValue = -99.99f;
// global attributes:
               :references = "Keeling etal1996, Keeling etal1995";
```

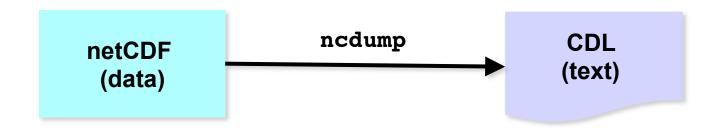
- "-h" is for "header only", just outputs metadata, no data
- "-c" outputs header and coordinate variable data
- ncgen does the opposite of ncdump, converts CDL to netCDF





# The ncdump utility

**ncdump** converts netCDF data to human-readable text form. Useful for browsing data, has lots of options.



**ncdump** [-c|-h] [-v ...] [-k] *file.nc* 

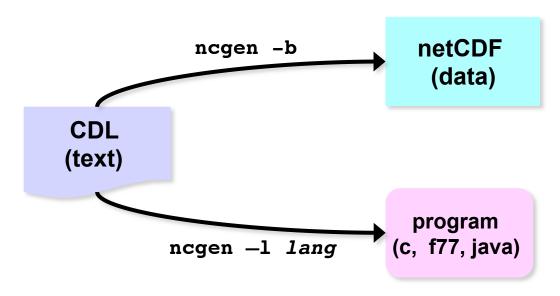
[-h | -c] header only, or coordinates and header [-v var1 [,...]] data for variable(s) var1,... only output kind of netCDF file instead of CDL show time data as date-time name of netCDF input file or OPeNDAP URL





# The ncgen utility

**ncgen** generates a netCDF file, or a program to generate the netCDF file.



**ncgen** [-b] [-o file.nc] [-k kind] [-l c|java] file.cdl

[-o file.nc] [-k kind] file.cdl

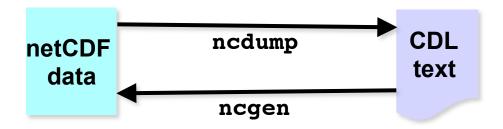
binary output as a netCDF file, with ".nc" extension like -b except output netCDF to specified file kind of output netCDF file, simplest that works if omitted [-l c|f77|java] language of program generated to standard output name of input CDL file



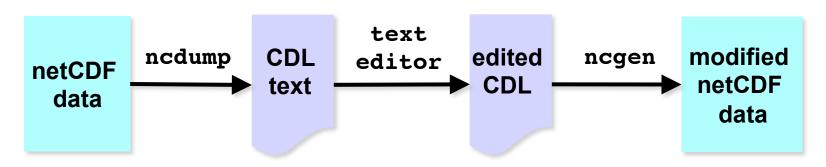


# Using ncgen and ncdump together

Together, **ncdump** and **ncgen** can accomplish simple manipulations with no programming. **ncdump** and **ncgen** are inverses:



To edit metadata or data in a netCDF file:



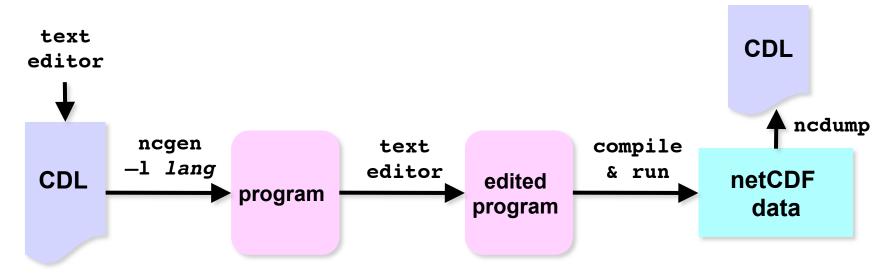
Note: not practical for huge netCDF files or lots of files. For that, you need to write a program, using netCDF library.





#### More of using ncgen and ncdump together

To create a new netCDF file with lots of metadata:



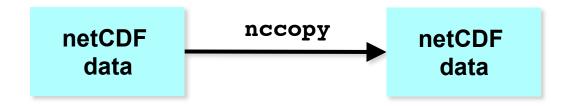
- 1. Use text editor to write CDL file with lots of metadata but no data.
- 2. Use **ncgen** to generate C or Fortran program for writing netCDF.
- 3. With text editor, insert netCDF "var\_put" calls for writing data.
- 4. Compile and run the program to create desired netCDF file.
- 5. Optionally, use **ncdump** to verify result.





# The nccopy utility

**nccopy** copies and optionally compresses and chunks netCDF data.



**nccopy** [-k kind] [-u] [-d level] [-s] [-c chunkspec] input output

[-k *kind*] kind of output netCDF, default same as input

[-u] convert unlimited dimensions to fixed-size in output

[-d level] zlib "deflation" level, default same as input

[-s] shuffling option, sometimes improves compression

[-c chunkspec] specify chunking for dimensions

input name of input file or OPeNDAP URL

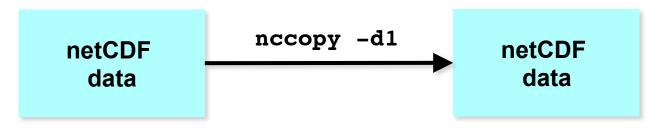
output name of output file



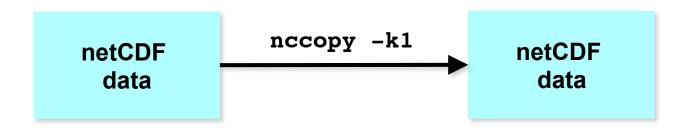


# Using nccopy

Compress netCDF data to a specified level, compressing each variable separately.



Convert a netCDF-4 classic model file to a netCDF-3 classic file, uncompressing any compressed variables.







# netCDF exercises





# Sample files for exercises

- Small netCDF file: data/mslp.nc
- Test file for compression: data/testrh.nc
- You can run netCDF utilities in iPython using "!" prefix, as in
   >>> !ncdump file.cdl
- Here's an example of capturing the output of a command (as a list of strings) into a python variable using assignment, and writing the list of output strings, separated by newlines, to a file:

```
>>> f = open('file.cdl', 'w')
>>> output_string = !ncdump file.nc
>>> f.write(output_string.n)
```





# Try ncdump utility

- Look at just the header information (also called the schema or metadata):
  - \$ ncdump -h mslp.nc
- Store entire CDL output for use later in ncgen exercises
   \$ ncdump mslp.nc > mslp.cdl
- Look at header and coordinate information, but not the data: \$ ncdump -c mslp.nc
- Look at all the data in the file, in addition to the metadata: \$ ncdump mslp.nc
- Look at a subset of the data by specifying one or more variables: \$ ncdump -v lat,time mslp.nc
- Look at times in human-readable form: \$ ncdump -t -v lat,time mslp.nc
- Look at what kind of netCDF data is in the file (classic, 64-bit offset, netCDF-4, or netCDF-4 classic model):
   \$ ncdump -k mslp.nc





#### Try ncgen utility

- Check a CDL file for any syntax errors:
   \$ ncgen mslp.cdl
- Edit mslp.cdl and change something (name of variable, data value, etc.).
- Use ncgen to generate new binary netCDF file (my.nc) with your changes:
  - \$ ncgen -o my.nc mslp.cdl
  - \$ ncdump my.nc
- Generate a C, Fortran, or Java program which, when compiled and run, will create the binary netCDF file corresponding to the CDL text file.
  - \$ ncgen -l c mslp.cdl > mslp.c
  - \$ ncgen –l f77 mslp.cdl > mslp.f77
  - \$ ncgen —l java mslp.cdl > mslp.java
- Try compiling and running one of those programs. You will need to know where the netCDF library is to link your program.





#### Try nccopy utility

• Compress variables in a test file, test.nc, by using nccopy. Then check if adding the shuffling option improves compression:

```
$ nccopy -d1 test.nc testd1.nc  # compress data, level 1
$ nccopy -d1 -s test.nc testd1s.nc  # shuffle and compress data
$ ls -l test.nc testd1.nc testd1s.nc  # check results
```

 Download just the variable named "Total\_precipitation" and relevant metadata from an OPeNDAP server dataset into a netCDF file named precip.nc

```
$ REMOTE_DIR=http://thredds.ucar.edu/thredds/dodsC/fmrc/NCEP/GFS/
Hawaii 160km
```

```
$ nccopy $REMOTE_DIR/NCEP-GFS-Hawaii_160km_best.ncd?Total_precipitation
precip.nc
```





#### Try remote access

- Look at what's in some remote data from an OPeNDAP server:
  - \$ REMOTE=http://test.opendap.org/opendap/data/nc/
    3fnoc.nc
  - \$ ncdump -c \$REMOTE
- Copy 3 coordinate variables out of the file
  - \$ nccopy "\${REMOTE}?lat,lon,time" coords.nc
- Copy subarray of variable u out of the file into a new netCDF file
  - \$ nccopy "\${REMOTE}?u[2:5][0:4][0:5]" U.NC
  - \$ ncdump u.nc





# Join the netCDF community

- Why participate?
  - To help extend netCDF to meet an important need.
  - To fix a bug that affects you or your users.
  - To help the geosciences community.
- How to collaborate?
  - Join netcdfgroup@unidata.ucar.edu mailing list
  - Use Unidata netCDF GitHub repository.
  - Build and test release candidates, provide feedback.
  - Contribute code, tests, and documentation improvements.
  - Suggest new features.
  - Also see netCDF Jira site for current open issues.



