# Introduction to netCDF formats, data models, and utilities

Russ Rew, UCAR Unidata
Workshop on Using Unidata Technologies with Python
21-22 October 2014

# 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

# 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 3rd-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

# NetCDF Compatibility Certificate

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
  - 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
  - Unidata supports and maintains C and Java implementations.
  - Unidata provides best-effort support for Fortran and C++ implementations.
  - Open source community and 3rd parties support and maintain other APIs, including netcdf4-python for Python.

# netCDF formats

# Characteristics of netCDF formats I

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

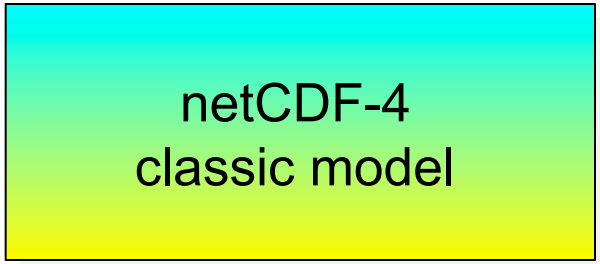
- ✓ Efficient compression from HDF5 storage
- ✓ Efficient access with HDF5 chunking
- ✓ Efficient schema changes supported
- ✓ Variables can be huge
- ✓ Good testing and support for high performance computing platforms

## 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"


- Compatible with existing applications
- Simplest data model and API



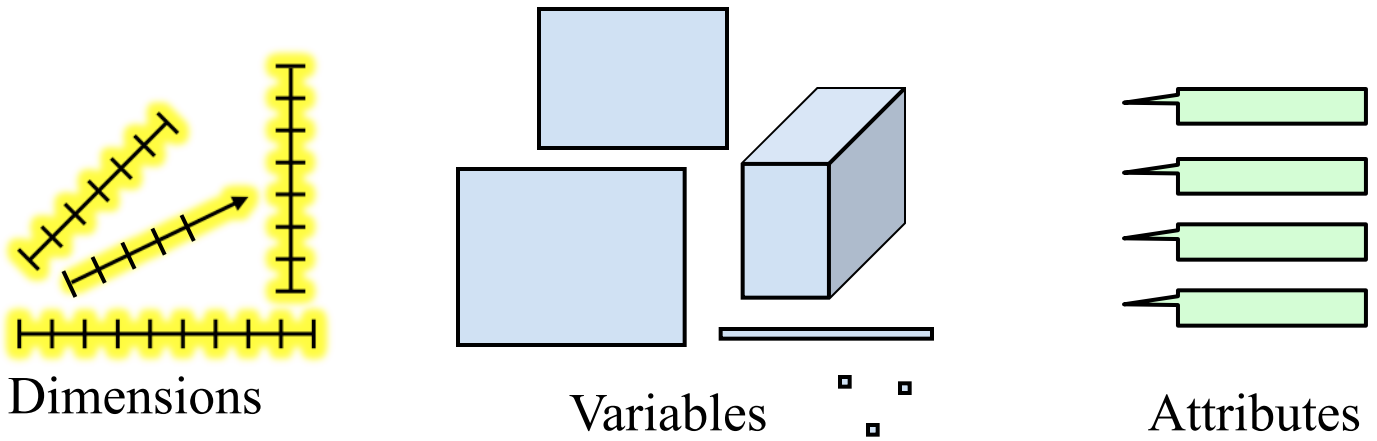

- Can be accessed through netCDF-3 APIs, compatible with classic data model
- Uses netCDF-4/HDF5 storage for performance: compression, chunking, …
- Transparent access after library update


- 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

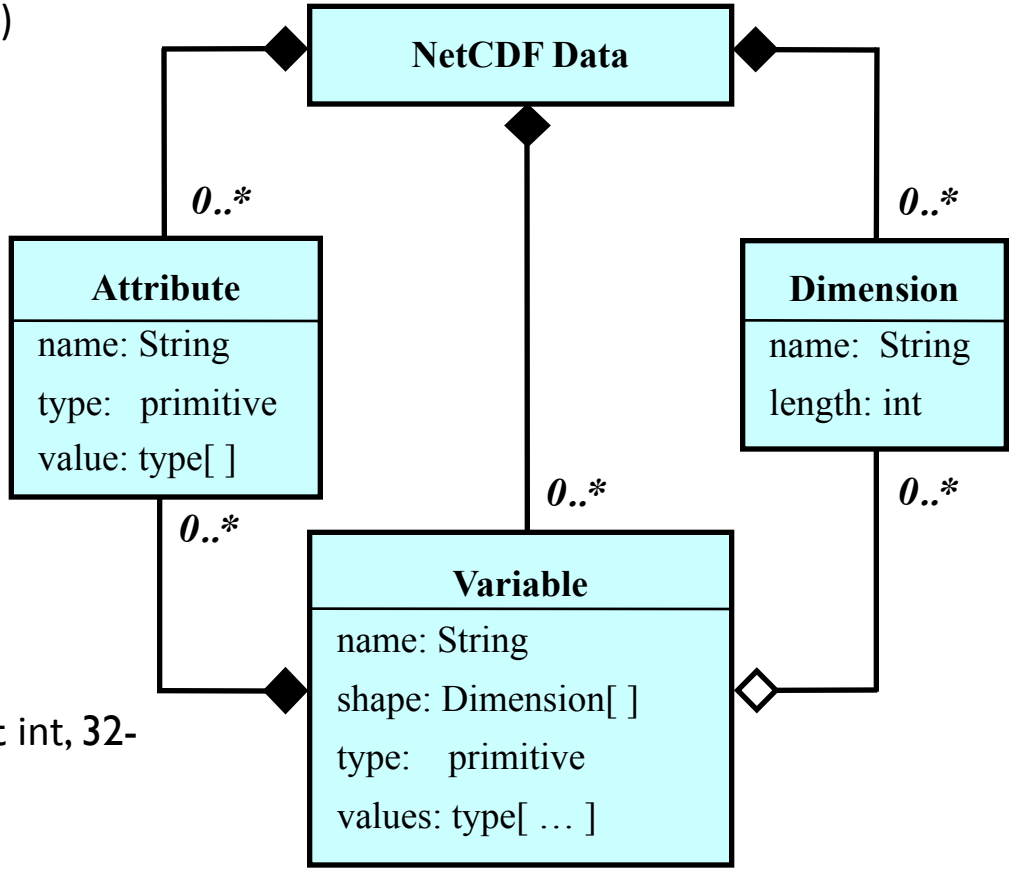
Each variable has
- Name, shape, type, attributes
- N-dimensional array of values

Each attribute has
- Name, type, value(s)

Variables may share dimensions
- Represents shared coordinates, grids

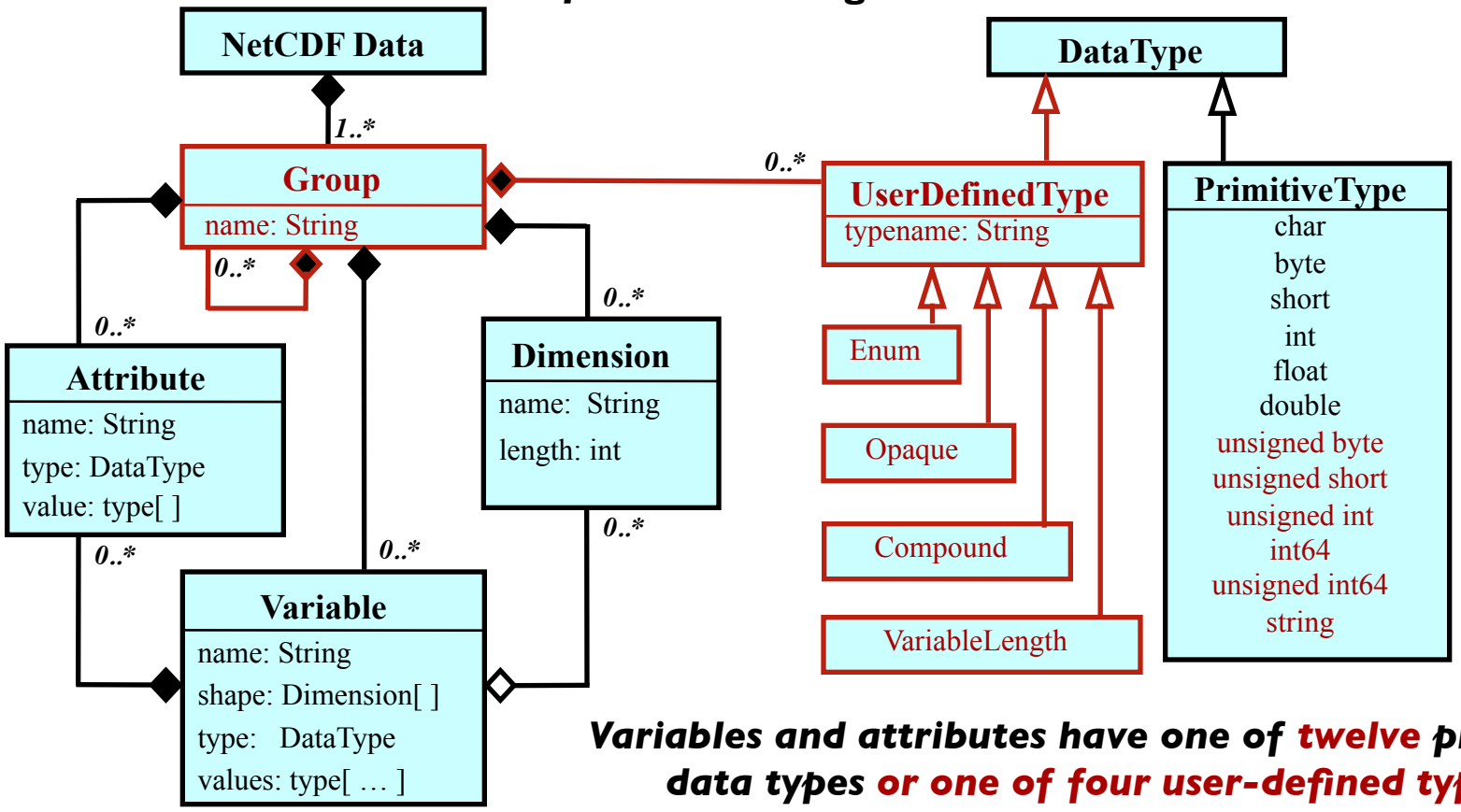
Variable and attribute values are of type
- Numeric: 8-bit byte, 16-bit short, 32-bit int, 32-bit float, 64-bit double
- Character: arrays of char for text

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 and attributes have one of twelve primitive data types or one of four user-defined types.***

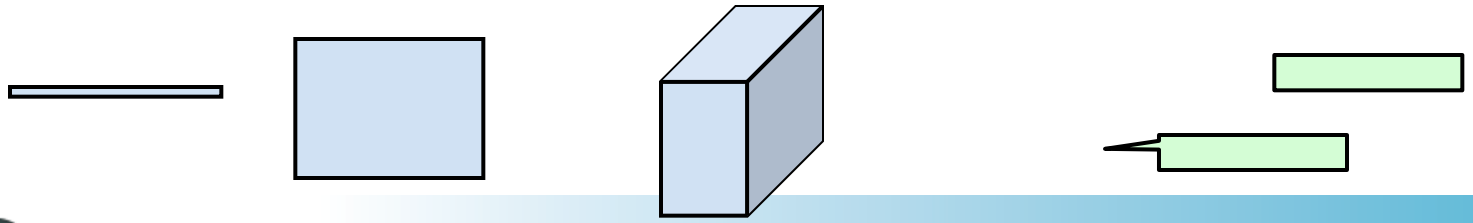
# Variables or attributes?

## 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

## Attributes

- 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
```

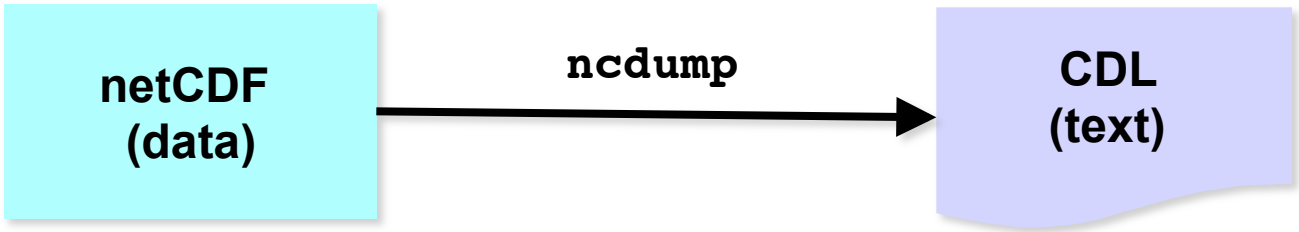
```
netcdf co2 {
dimensions:
        T = 456 ;
variables:
        float T(T) ;
                T:units = "months since 1960-01-01" ;
        float co2(T) ;
                co2:long_name = "CO2 concentration by volume" ;
                co2:units = "1.0e-6" ;
                co2:_FillValue = -99.99f ;

// 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.

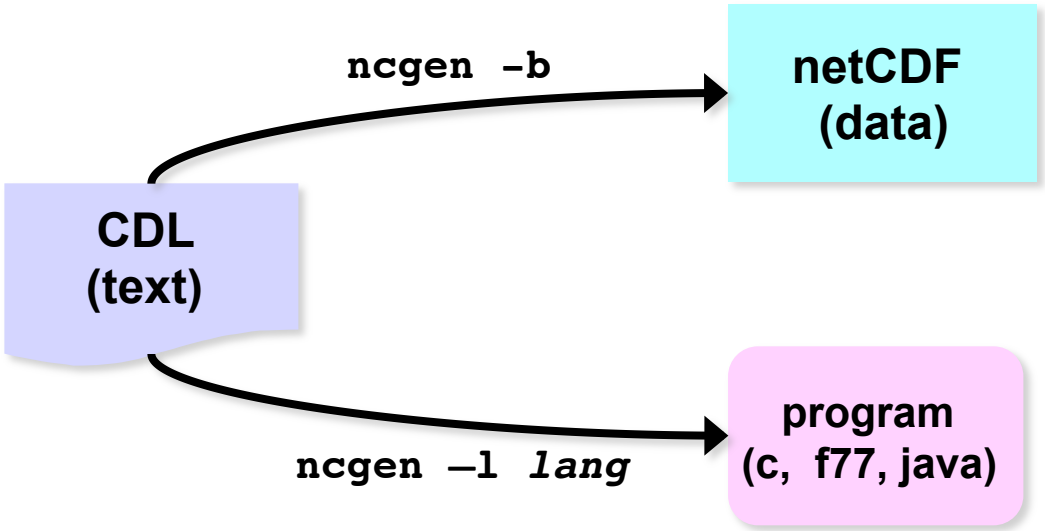



**ncdump** [-c|-h] [-v ...] [-k] *file.nc*

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

# The ncgen utility

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

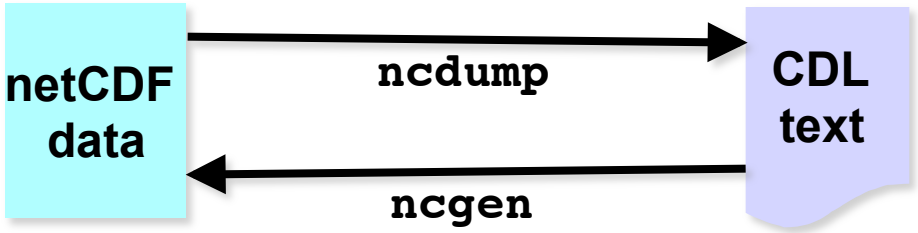



**ncgen** [-b] [-o file.nc] [-k *kind*] [-l c | java] *file.cdl*

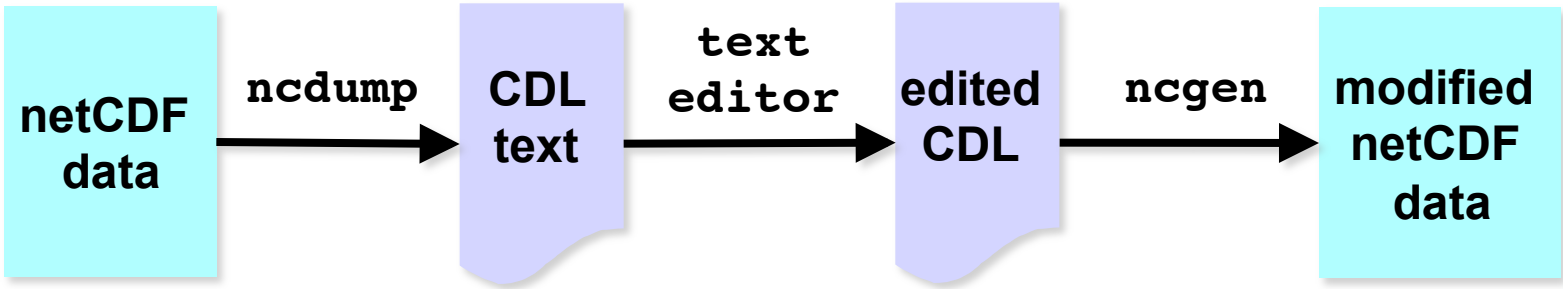
| | |
|---|---|
| [-b] | binary output as a netCDF file, with ".nc" extension |
| [-o *file.nc*] | like -b except output netCDF to specified file |
| [-k *kind*] | kind of output netCDF file, simplest that works if omitted |
| [-l c \| f77 \| java] | language of program generated to standard output |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



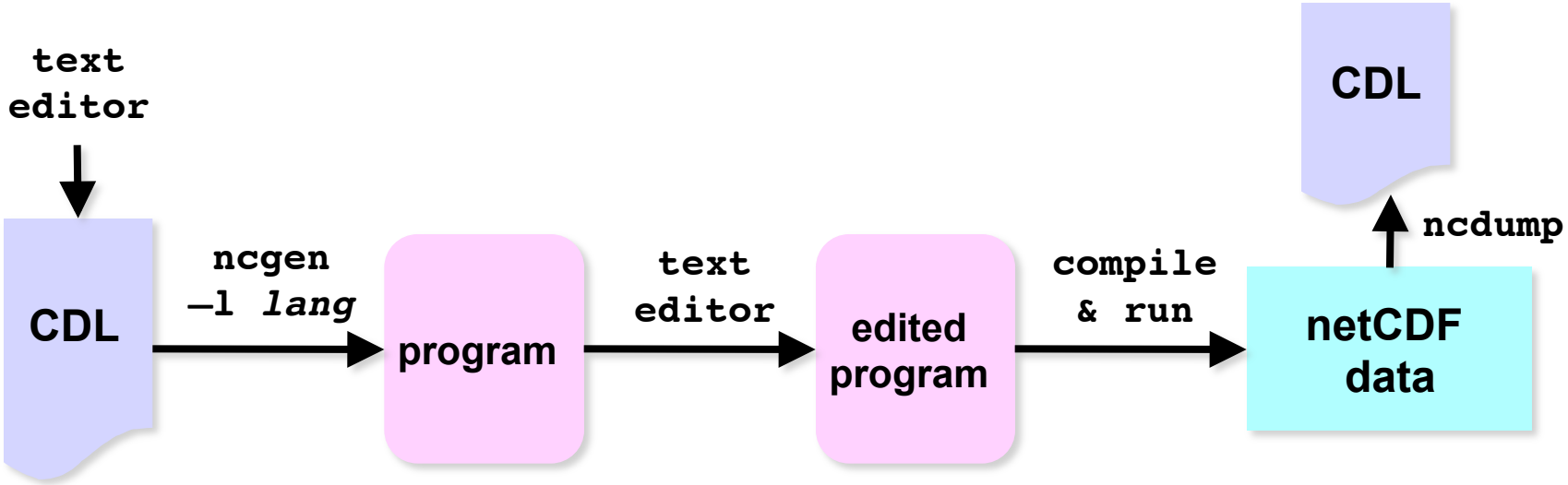

To edit metadata or data in a netCDF file:




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

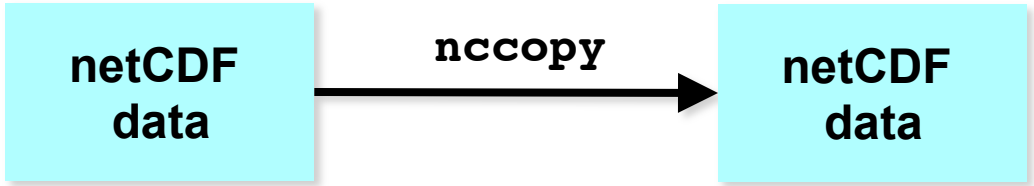
To create a new netCDF file with lots of metadata:




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.

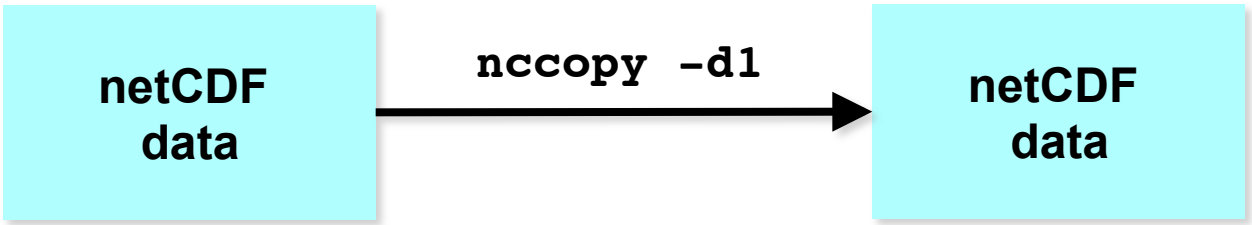



**nccopy** [-k *kind*] [-u] [-d *level*] [-s] [-c *chunkspec*] *input* *output*

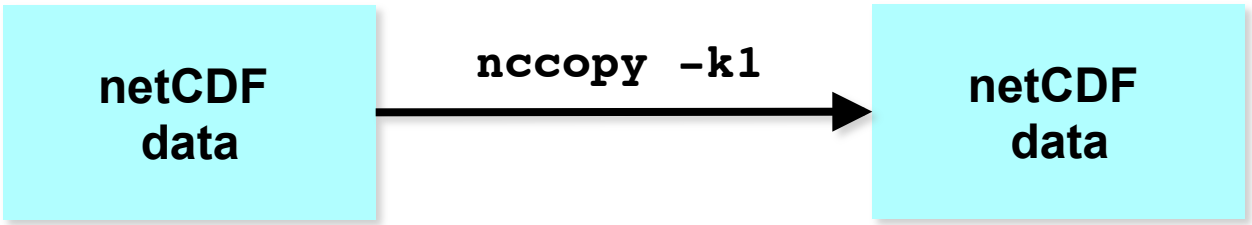
[-k *kind*] kind of output netCDF, default same as input
[-u] convert unlimited dimensions to fixed-size in output
[-d *level*] zlib "deflation" level, default same as input
[-s] shuffling option, sometimes improves compression
[-c *chunkspec*] specify chunking for dimensions
*input* name of input file 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.nc
```

- 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)
>>> f.close()
```

# 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 remote access

- Look at what's in some remote data from an OPeNDAP server:

```
$ SERVER=http://test.opendap.org
$ REMOTE=$SERVER/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
```

# Try compression with nccopy utility

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

```
$ nccopy -d1 testeh.nc testrhd1.nc        # compress data, level 1
$ nccopy -d1 -s testrh.nc testrhd1s.nc    # shuffle and compress data
$ ls -l testrh.nc testrhd1.nc testrhd1s.nc  # check results
```

# 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.