Unidata

Providing data services, tools, & cyberinfrastructure leadership that advance Earth system science, enhance educational opportunities, & broaden participation

Introduction to NetCDF

Russ Rew, UCAR Unidata
ICTP Advanced School on High Performance and Grid Computing
13 April 2011









Overview

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



Background: What is Unidata?

- Where netCDF is developed and maintained
- Funded primarily by US National Science Foundation through UCAR
- Staff of about 22, including 13 developers
- Mission: data services, tools, and community leadership to advance Earth system science, enhance educational opportunities, and broaden participation
- Open source software for data access and distribution, analysis and visualization, community advocacy, workshops, and software support



What is netCDF?



NetCDF History



1988: NetCDF developed at Unidata



1996: NetCDF v3.0 new API



2008: NetCDF v4.0 uses HDF5

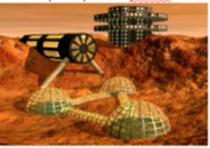
1991: NetCDF v2.0 new API



2004: NetCDF v3.6.0 64-bit offset format



2010: NetCDF v4.1.1 opendap/HDF4/pnetcdf





NetCDF: not just a format

*net*work *C*ommon *D*ata *F*orm

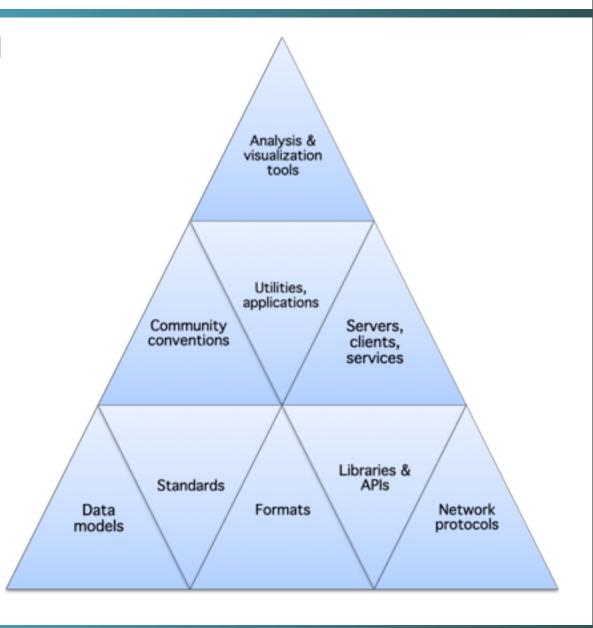
- Data model for scientific data and metadata
 - Widely used in ocean, climate, atmospheric science
 - Used in some other disciplines: molecular dynamics, neuro-imaging, fusion research ...
- File format for portable data
 - Array-oriented scientific data and metadata
 - NetCDF data is self-describing, portable, direct access, appendable, networkable, extensible, sharable, archivable
- Application programming interfaces (APIs)
 - C, Java, C++, Fortran (Developed and supported by UCAR / Unidata)
 - Python, Ruby, Perl, MATLAB, IDL, ...
 (3rd party APIs)

Together, the data model, file format, and APIs support the creation, access, and sharing of scientific data



Infrastructure for sharing scientific data

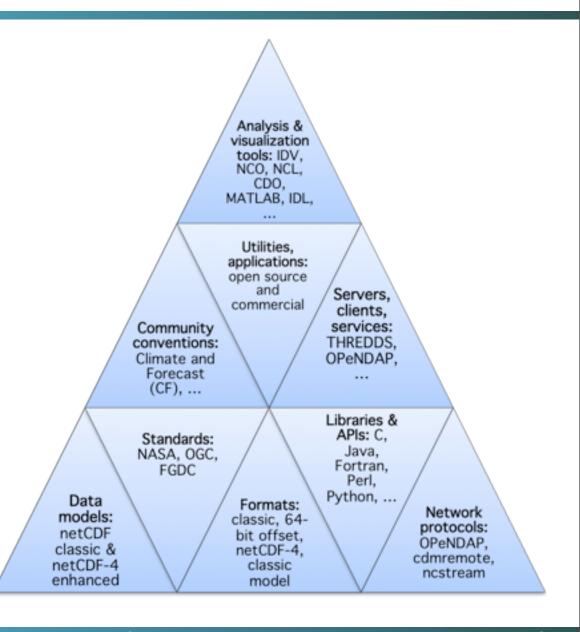
- Applications depend on lower layers
- Sharing requires agreements
 - formats
 - protocols
 - conventions
- Data needs metadata
- Is all this infrastructure really necessary?





NetCDF infrastructure

- Provides format and library for netCDF data model
- Endorsed by several standards bodies
- Active conventions communities
- OPeNDAP protocol
- Several servers for remote data access
- Many open source and commercial utilities and applications





www.unidata.ucar.edu/netcdf/



Development Milestones

1989: portable, self-describing data format, data model, and software for creation, access, and sharing of scientific data

1990's: growth of use in ocean and climate models, 3rd-party software support (NCO, NCL, IDL, MATLAB)

2002: Java version with OPeNDAP client support

2003: NASA funded netCDF-4/HDF5 project; Argonne/ Northwestern parallel netCDF

2004: netCDF-Java plug ins for reading other formats, NcML aggregation service

2007: netCDF-Java Common Data Model (access to other formats through netCDF interface)

2008: netCDF-4 C and Fortran library with HDF5 integration, enhanced data model, parallel I/O

2009: "netCDF classic format" becomes NASA standard

2010: version 4.1.1 - OPeNDAP client support for C/Fortran libraries; udunits, CF library support; pnetcdf, HDF4 access, FGDC standardization

2011: version 4.1.2 – speedups, refactoring, bug fixes, new functions, nccopy supports compression and chunking, OGC standardization, Windows version





Who uses netCDF?

- Climate modelers
 - Program for Climate Model Diagnosis and Intercomparison (PCMDI)
 - Earth Systems Grid
- Ocean and atmospheric sciences
 - Forecast models
 - Atmospheric chemistry
- Neuroimaging
 - MINC Medical Image NetCDF
 - NiBabel
- Fusion research
 - Culham Centre for Fusion Energy (C++ API for netCDF-4)
- Molecular dynamics simulations (e.g. AMBER)



NetCDF standards endorsements

- 2009-02-05: NASA Earth Science Data Systems (ESDS) Standards Process
 Group endorsed netCDF classic and 64-bit offset formats as appropriate
 for NASA Earth Science data.
- 2010-03-1: Integrated Ocean Observing System (IOOS) Data
 Management and Communications (DMAC) Subsystem endorsed netCDF
 with Climate and Forecast (CF) conventions as a preferred data format.
- 2010-09-27: Steering Committee of the US Federal Geographic Data Committee (FGDC) officially endorsed **netCDF** as a Common Encoding Standard.
- 2011-03-07: Open Geospatial Consortium (OGC) approved "OGC
 Network Common Data Form (NetCDF) Core Encoding Standard version
 1.0" as a new OGC standard. Thanks to Dr. Ben Domenico (Unidata) and
 Dr. Stefano Nativi (University of Florence, CNR-IMAA).





PER L'ANALISI AMBIENTALE



Data models and formats



What is a data model?

Formally:

- A collection of data objects such as lists, tables, relations, ...
- A collection of operations that can be applied to the objects such as retrieval, update, subsetting, averaging, ...
- A collection of integrity rules that define the legal states (set of values) or changes of state (operations on values)
- We won't be that formal, will just draw pictures and wave our hands
 - to describe what netCDF data objects are and what you can do with them
 - independent from data format details
 - independent from programming language



Data model examples

- Relational data model
 - Concepts: tables, rows, columns, types
 - Operations: create, replace, update, delete, find, index, ...
 - Rules: normal forms, integrity constraints

| Name | Email | Role | ID# |
|-------|----------------|---------|-----|
| Alice | alice@univ.edu | Student | 123 |
| Bob | bob@abc.com | Student | 456 |

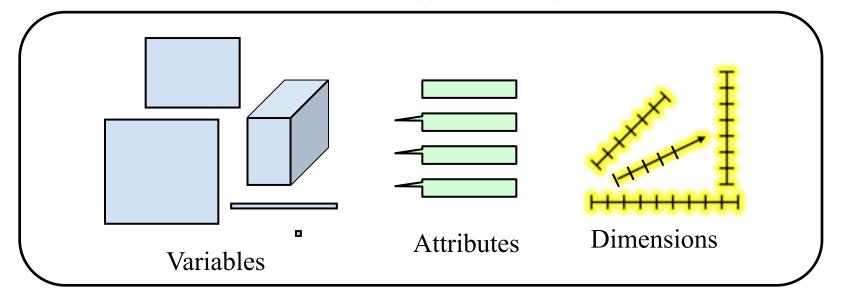
- Geospatial information system data model
 - Concepts: locations, lines, polygons, features, surfaces
 - Operations: create, replace, update, delete, intersects
 - Rules: adjacent features share a common edge, ...





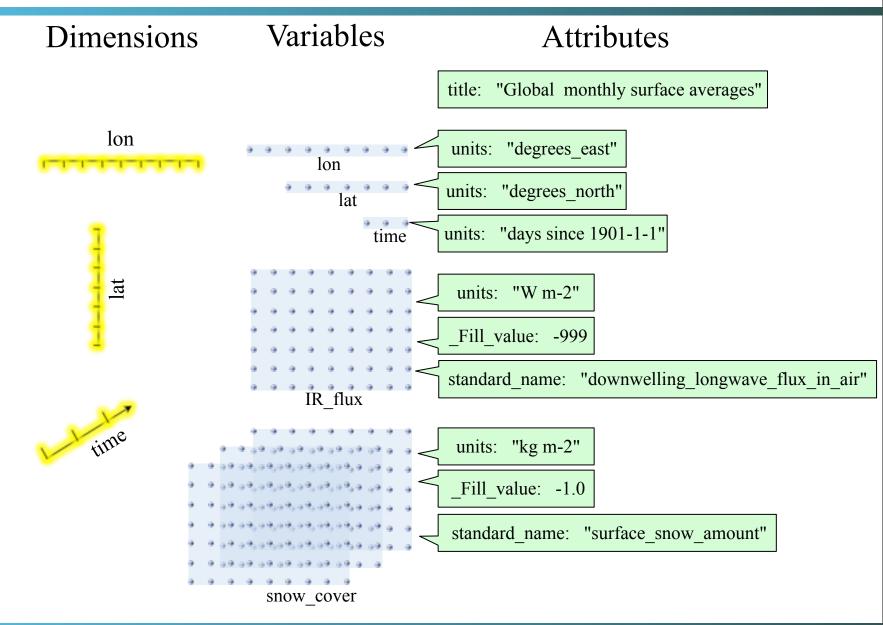
The netCDF "classic" data model, in words

- A netCDF file has named variables, attributes, and dimensions.
- Variables are for data, attributes are for metadata (data about data)
- Dimensions are for specifying shapes of variables
- Attributes may apply to a whole file or to a single variable
- Variables may share dimensions, indicating a common grid.
- One dimension may be of unlimited length.
- Each variable or attribute has 1 of 6 types: char, byte, short, int, float, double





Example of netCDF classic data model





The netCDF classic data model, in UML

NetCDF Data has

Variables (eg temperature, pressure)

Attributes (eg units)

Dimensions (eg lat, lon, level, time)

Each variables has

Name, shape, type, attributes

N-dimensional array of values

Each attributes has

Name, type, value(s)

Each dimensions has

Name, length

Variables *may share* dimensions

Represents shared coordinates, grids

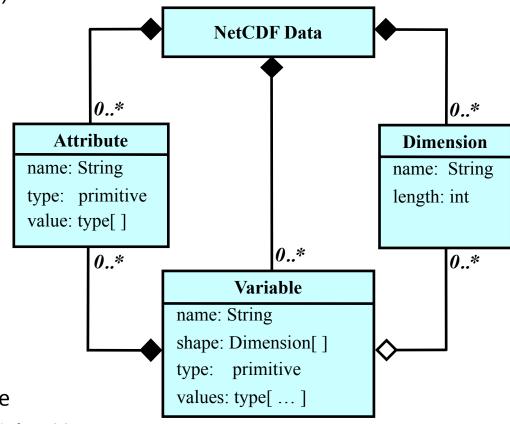
Variable and attribute values are of type

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





Common Data Language (CDL)

Text notation for netCDF metadata and data

```
netcdf snow{ // example of CDL notation
 dimensions:
   lon= 9 ;
   lat= 7 ;
   time = unlimited ; // 3 currently
 variables:
   float IR flux(lon, lat);
     IR flux:units = "W m-2" ;
     IR flux:_Fill_value = -999 ;
     IR flux:standard name= "downwelling longwave flux in air";
   float snow cover(time, lon, lat);
     snow cover:units = "kg m-2";
 // global attributes
         :title = "simple example, lacks some conventions";
 data:
  IR flux = 200, 201, ...;
  snow cover = 0.1, 0.2, 0.0, ...;
}
```



NetCDF format characteristics

- **Self-Describing:** A netCDF file includes metadata as well as data: names of variables, data locations in time and space, units of measure, and other useful information.
- Portable: Data written on one platform can be read on other platforms.
- **Direct-access:** A small subset of a large dataset may be accessed efficiently, without first reading through all the preceding data.
- Appendable: Data may be efficiently added to a netCDF file without copying the dataset or redefining its structure.
- **Extensible:** Adding new dimensions, variables, or attributes to netCDF files does not require changes to existing programs that read the files.
- Sharable: One writer and multiple readers may simultaneously access the same netCDF file. With Parallel netCDF, multiple writers may efficiently and concurrently write into the same netCDF file.
- **Archivable:** Access to all earlier forms of netCDF data will be supported by current and future versions of the software.
- **Networkable:** The netCDF library provides client access to structured data on remote servers through OPeNDAP protocols.



NetCDF classic data model

Strengths

- ✓ Data model simple to understand and explain
- ✓ Efficient implementation freely available
- ✓ Generic applications easy to develop
- Representation good for gridded multidimensional data
- ✓ Shared dimensions useful for coordinate systems

Limitations

- Small set of primitive types
- Flat data model limited to multidimensional arrays, lists, (name, value) pairs
- Flat name space not ideal for organizing many data objects
- Lacks nested structures, variable-length types, enumerations



NetCDF classic format

Strengths

- ✓ Simple to understand and explain
- ✓ Supported by many applications
- ✓ Standard used in many archives, data projects
- ✓ Mature conventions and best practices have evolved

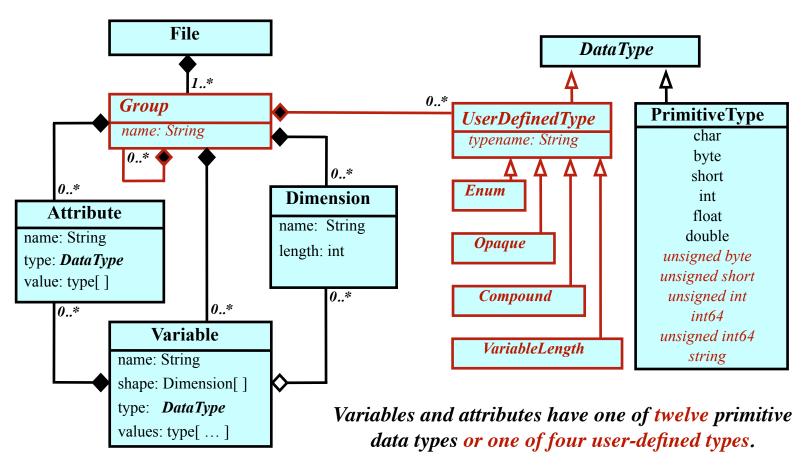
Limitations

- No support for efficient compression
- Only one dimension can grow efficiently
- Portable representation favors big-endian platforms
- Schema changes can be costly



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.





NetCDF enhanced data model

Strengths

- ✓ Simpler than HDF5, with similar representational power
- ✓ Adds shared dimensions to HDF5 data model
- ✓ Continues support for existing data, software, and conventions
- ✓ Eliminates netCDF classic model limitations
- ✓ Provides nested structures: hierarchical groups, recursive data types
- ✓ Independent features permit incremental adaptation, adoption

On the other hand

- More complex than classic data model
- More effort required to develop general tools and applications
- Not yet widely adopted
- Hence, no comprehensive best practices and conventions yet



NetCDF-4 format

- Uses HDF5 as a storage layer
- Provides performance advantages of HDF5
 - Compression
 - Chunking
 - Parallel I/O
 - Efficient schema changes
- Useful for larger or more complex datasets
- Suitable for high-performance computing





NetCDF-4 classic-model: a transitional format

netCDF-3

- Compatible with existing applications
- Simplest data model and API

netCDF-4 classic model

- Uses classic API for compatibility
- Uses netCDF-4/HDF5 storage for compression, chunking, performance
- To use, just recompile, relink

netCDF-4

- Not compatible with some existing applications
- Enhanced data model and API, more complex, powerful



Common Data Language (CDL), again

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 some conventions";
 data:
  rh =
   2, 3, 5, 7, 11, 13, 17, 19,
   23, 29, 31, 37, 41, 43, 47, 53;
}
```

A netCDF file with 2 dimensions (x and y), 1 variable (rh), 2 variable attributes (units and long_name), 1 global attribute (title), and some data values.



Utility programs for netCDF to/from CDL

\$ ncdump -h co2.nc

```
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
- The ncgen utility does the opposite of ncdump, converts CDL to netCDF



Coordinate variables convention

Coordinate variables

- have same name as a dimension
- contain coordinate values for the dimension
- should be one-dimensional
- should contain no missing values
- should have values that are strictly increasing or strictly decreasing

```
dimensions:
 lon=9;
 lat= 7 :
 time = unlimited; // 3 currently
variables:
 float lon(lon);
   lon:units = "degrees east" ;
 float lat(lat);
   lat:units = "degrees north" ;
 int time(time) ;
    time:units = "days since 2011-1-1";
data:
 lon = -154.3, -102.9, \dots, 154.3;
 lat = -90, -60, ..., 90;
 time = 10, 20, 30;
```

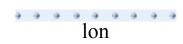
Dimensions:



lon time

Coordinate variables:







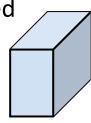


Variables or attributes?

Variables

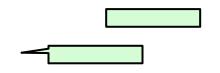
- intended for data
- can hold arrays too large for memory
- may be multidimensional
- support partial access (only a subset of values)
- values may be changed, more data may be appended
- may have attributes
- shape specified with netCDF dimensions
- not read until accessed





Attributes

- intended for metadata
- for small units of information that fit in memory
- for single values, strings, or small1-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



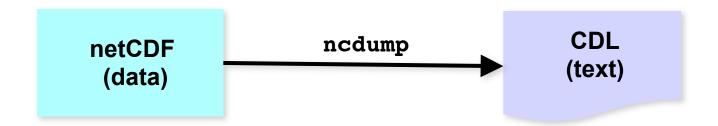


Utilities: ncdump, ncgen, nccopy



The ncdump utility

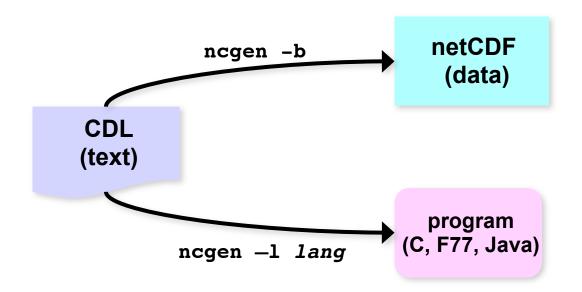
- Converts netCDF data to human-readable text form
- Useful for browsing data files





The ncgen utility

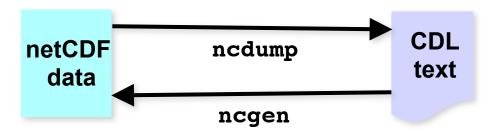
- Converts netCDF CDL to a binary netCDF file or a program
- Useful for generating netCDF files without programming



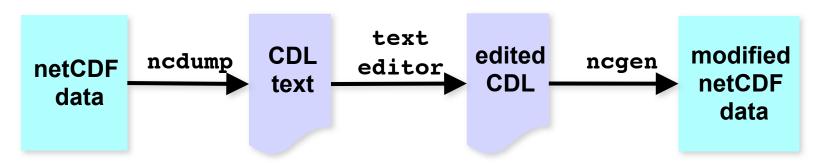


Using ncgen and ncdump together

The ncdump and ncgen utilities are inverses of each other:



To add, delete, or change metadata or data in a netCDF file:

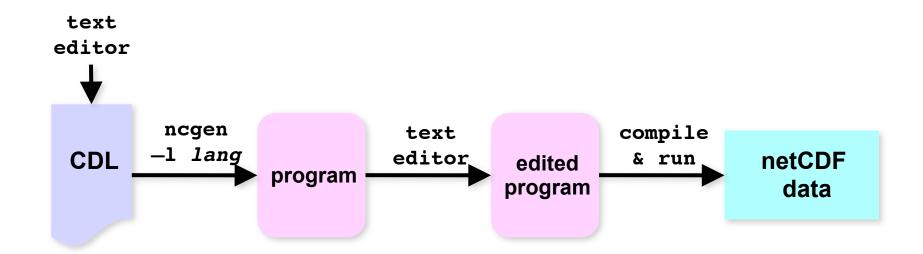


This is not very practical for huge files or a large number of files.
 In that case you may need to write a program, using the netCDF library.



More of using ncgen and ncdump together

To create a new netCDF file with lots of metadata:

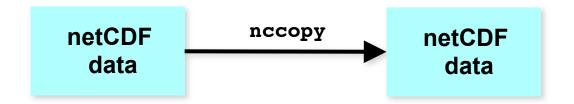


- Insert easy "var_put(...)" calls to the netCDF library for the data writing part of the task
- Compile and run the program to create desired netCDF file
- Use ncdump to verify the desired file is created.



The nccopy utility

- Copies or converts and optionally compresses netCDF data
- Can also "re-chunk" data for more optimized access





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.





The nc-config utility

- nc-config reports on version installed and assists with setting compiler and linker flags for applications
- To compile and link a C application and a Fortran application, using nc-config:

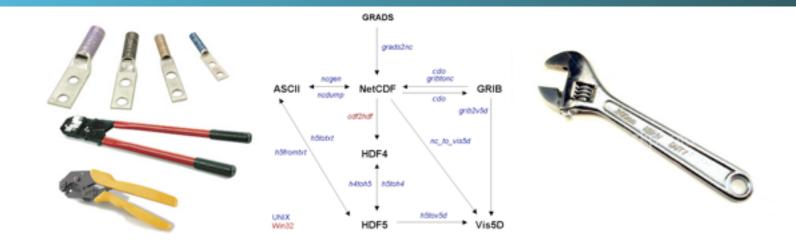
```
$ cc `nc-config --cflags` myapp.c -o myapp `nc-config --libs`
$ f95 `nc-config --fflags` yrapp.f -o yrapp `nc-config --flibs`
```

 To report all the features of the netCDF installation you are using (support for remote access clients, netCDF-4, parallel IO, HDF4 access support, etc.)

```
nc-config --all
```



Other netCDF utilities and applications



- Many other useful netCDF utilities developed by third parties are available, including both open source (e.g. NCL, NCO, CDO) and commercial (MATLAB, IDL, ARCInfo) packages.
- For information about over 100 such packages, consult Unidata's <u>Software for Manipulating or Displaying NetCDF Data</u> or ARM's <u>list</u> <u>of data tools</u>, which includes some downloadable binaries.



More information

Online netCDF workshop

www.unidata.ucar.edu/netcdf/workshops/2010/

Software support:

support-netcdf@unidata.ucar.edu

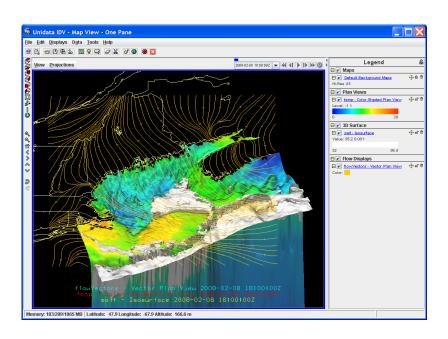
 Software tools for manipulating or displaying netCDF data:

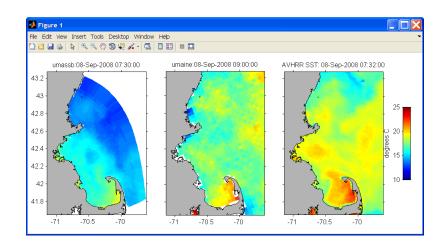
www.unidata.ucar.edu/netcdf/docs/software.html

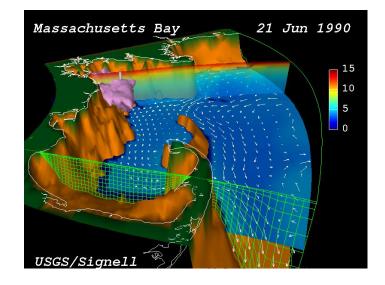


Questions?











Exercises



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 -I 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

(Requires netCDF version 4.1.2 or later)

 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

```
$ nccopy \
'http://motherlode.ucar.edu/thredds/dodsC/fmrc/NCEP/GFS/\
Hawaii_160km/NCEP-GFS-Hawaii_160km_best.ncd?Total_precipitation' \
precip.nc
```



Try remote access

(Requires netCDF built with DAP support, vers. 4.1.1 or later)

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

```
$ ncdump -c http://test.opendap.org/opendap/data/nc/
3fnoc.nc
```

Copy 3 coordinate variables out of the file

```
$ nccopy "http://test.opendap.org/opendap/data/nc/
3fnoc.nc?lat,lon,time" coords.nc
```

Copy subarray of variable u out of the file into a new netCDF file

```
$ nccopy "http://test.opendap.org/opendap/data/nc/3fnoc.nc?
u[2:5][0:4][0:5]" u.nc
$ ncdump u.nc
```