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Providing data, tools, and community leadership for enhanced Earth-system education and research

Writing NetCDF Files: Formats, Models, Conventions, and Best Practices

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Overview

- Formats, conventions, and models
- NetCDF-3 limitations
- NetCDF-4 features: examples and potential uses
- Compatibility issues
- Conventions issues
- Recommendations

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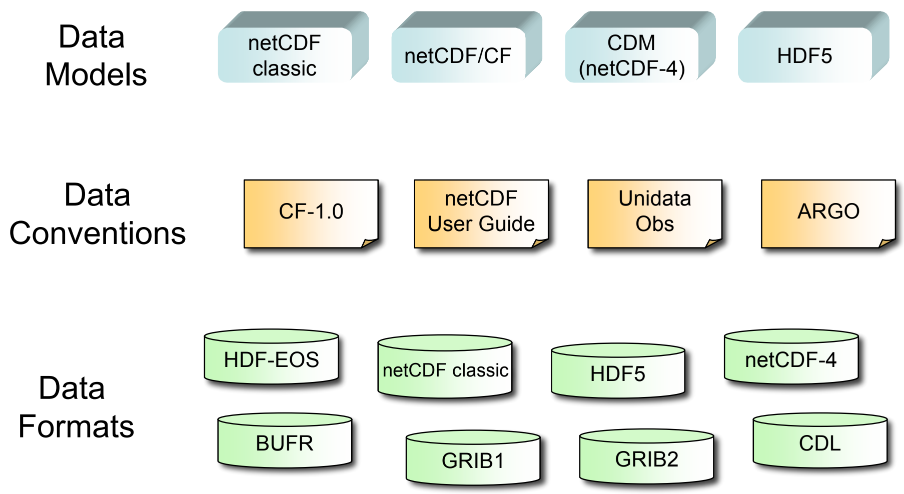
Data Abstraction Levels: Formats, Conventions, and Models



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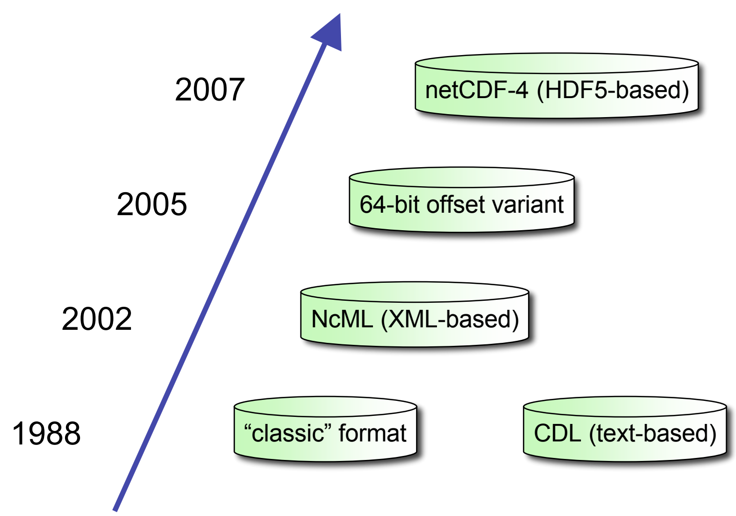
NetCDF Formats



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Commitment to Backward Compatibility

Because preserving access to archived data for future generations is sacrosanct :

- **Data access**: New netCDF software will provide read and write access to ***all*** earlier forms of netCDF data.
- **APIs and programs**: Existing C, Fortran, and Java netCDF programs will be supported by new netCDF software (possibly after recompiling).
- **Commitment**: Future versions of netCDF software will continue to support data access, API, and conventions compatibility.

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Purpose of Data Conventions

- To capture meaning in data
- To make files self-describing
- To faithfully represent intent of data provider
- To foster interoperability
- To add value to formats
  - Raise level of abstraction (e.g. adding coordinate systems)
  - Customize format for discipline or community (e.g. climate modeling)

CF-1.0 | netCDF User Guide | Unidata Obs | ARGO | ...

NetCDF conventions

- Users Guide conventions:
  - Simple coordinate variables (same name for dimension and variable)
  - Common attributes: **`units`**, **`long_name`**, **`valid_range`**, **`scale_factor`**, **`add_offset`**, **`_FillValue`**, **`history`**, **`Conventions`**, …
  - Not just for earth-science data
- Followed by lots of community conventions: COARDS, GDT, NCAR-RAF, ARGO, AMBER, PMEL-EPIC, NODC, …, CF
- Unidata Obs Conventions for netCDF-3 (supported by Java interface)
- Climate and Forecast conventions (CF) endorsed by Unidata (2005)
- Unidata committed to development of libcf (2006)

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CF Conventions (cfconventions.org)

- Clear, comprehensive, consistent (thanks to Eaton, Gregory, Drach, Taylor, Hankin)
- `standard_name` attribute for identifying quantities, comparison of variables from different sources
- Coordinate systems support
- Grid cell bounds and measures
- Acceptance by community: IPCC AR4 archive, …
- Governance and stewardship: GO-ESSP, BADC, PCMDI, WCRP/WGCM (pending)

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CF Conventions Issues

- cf-metadata mailing list
- cfconventions.org site: documents, forums, wiki, Trac system
- GO-ESSP annual meetings
- Recent CF issues and proposed CF extensions
  - Structured grids, staggered grids, subgrids, curvilinear coordinates (Balaji)
  - Unstructured grids (Gross)
  - Forecast time axis (Gregory, Caron)
  - Means and subgrid variation and anomaly modifier for standard names
  - Additions needed for observational data
  - NetCDF-4 issues
  - Needs for IPCC AR5 model output archives

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Scientific Data Models

- Tabular data
  - Relational model
  - Tuples, types, queries, operations, normalization, integrity constraints
- Geographic data
  - GIS models
  - Features and coverages, observations and measurements
  - Adds spatial location to relational model
- Multidimensional array data
  - Basis of netCDF, HDF models
  - Dimensions, variables, attributes
- Scientific data types
  - Coordinate systems, groups, types: structures, varlens, enums
  - N-dimensional grids, *in situ* point observations, profiles, time series, trajectories, swaths, …

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NetCDF Data Models

- "Classic" netCDF model (netCDF-3 and earlier)
  - Dimensions, Variables, and Attributes
  - Character arrays and a few numeric types
  - Simple, flat
- CDM (netCDF-4 and later)
  - Dimensions, Variables, Attributes, Groups, Types
  - Additional primitive types including strings
  - User-defined types support structures, variable-length values, enumerations
  - Power of recursive structures: hierarchical groups, nested types

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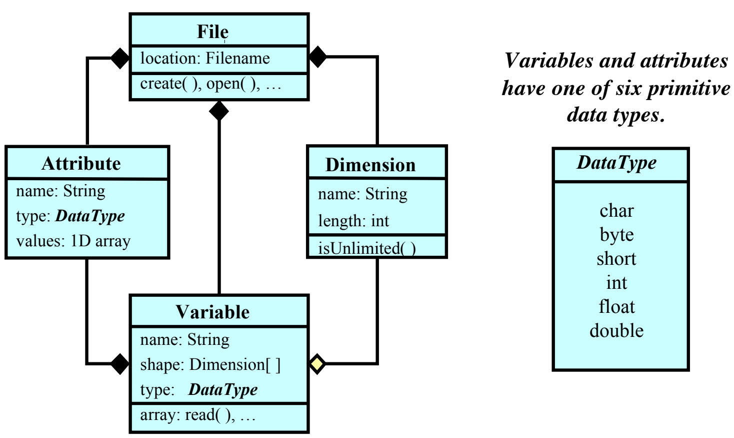
Classic NetCDF Data Model



A file has named variables, dimensions, and attributes. A variable may also have attributes. Variables may share dimensions, indicating a common grid. One dimension may be of unlimited length.

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Some Limitations of Classic NetCDF Data Model and Format

- Little support for data structures, just multidimensional arrays and lists
- No nested structures or “ragged arrays”
- Only one shared unlimited dimension for appending new data efficiently
- Flat name space for dimensions and variables
- Character arrays rather than strings
- Small set of numeric types
- Constraints on sizes of large variables
- No compression, just packing
- Schema additions may be *very* inefficient
- Big-endian bias may hamper performance on little-endian platforms

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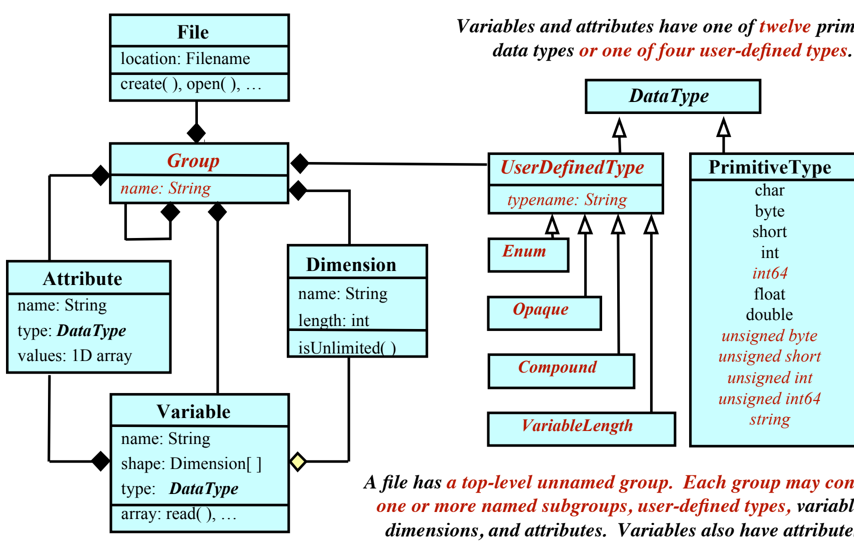
NetCDF-4 Data Model

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



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.

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NetCDF-4 Format and Data Model Benefits

HDF5-based format provides:

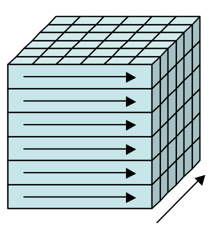
- Per-variable compression
- Per-variable multidimensional tiling (chunking)
- Ample variable sizes
- Reader-makes-right conversion
- Efficient dynamic schema additions
- Parallel I/O

New data model provides:

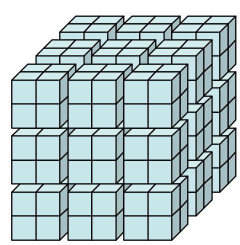
- Groups for nested scopes
- User-defined enumeration types
- User-defined compound types
- User-defined variable-length types
- Multiple unlimited dimensions
- String type
- Additional numeric types

Chunking

- Allows efficient access of multidimensional data along multiple axes
- Compression applies separately to each chunk
- Can improve I/O performance for very large arrays and for compressed variables
- Default chunking parameters are based on a size of one in each unlimited dimension



index order



chunked

NetCDF-4 Data Model Features

- Examples in “CDL-4”
  - Groups
  - Compound types
  - Enumerations
  - Variable-length types
- Not necessarily best practices
- Other potential known uses
- Advice on known limitations
- Potential conventions issues

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Example Use of Groups

Organize data by named property, e.g. region:

```
group Europe {
  group France {
    dimensions: time = unlimited, stations = 47;
    variables: float temperature(time, stations);
  }
  group England{
    dimensions: time = unlimited, stations = 61;
    variables: float temperature(time, stations);
  }
  group Germany {
    dimensions: time = unlimited, stations = 53;
    variables: float temperature(time, stations);
  }
  …
  dimensions: time = unlimited;
  variables: float average_temperature(time);
}
```

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Potential Uses for Groups

- Factoring out common information
  - Containers for data within regions, ensembles
  - Model metadata
- Organizing a large number of variables
- Providing name spaces for multiple uses of same names for dimensions, variables, attributes
- Modeling large hierarchies

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Example Use of Compound Type

Vector quantity, such as wind:

```
types:
  compound wind_vector_t {
    float eastward ;
    float northward ;
    }
dimensions:
    lat = 18 ;
    lon = 36 ;
    pres = 15 ;
    time = 4 ;
variables:
    wind_vector_t gwind(time, pres, lat, lon) ;
       wind:long_name = "geostrophic wind vector" ;
       wind:standard_name = "geostrophic_wind_vector" ;
data:
    gwind = {1, -2.5}, {-1, 2}, {20, 10}, {1.5, 1.5}, ...;
```

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Another Compound Type Example

Point observations :

```
types:
  compound ob_t {
      int station_id ;
      double time ;
      float temperature ;
      float pressure ;
  }
dimensions:
    nstations = unlimited ;
variables:
    ob_t obs(nstations) ;
data:
    obs = {42, 0.0, 20.5, 950.0}, … ;
```


Potential Uses for Compound Types

- Representing vector quantities like wind
- Modeling relational database tuples
- Representing objects with components
- Bundling multiple *in situ* observations together (profiles, soundings)
- Providing containers for related values of other user-defined types (strings, enums, …)
- Representing C structures portably
- CF Conventions issues:
  - should type definitions or names be in conventions?
  - should member names be part of convention?
  - should quantities associated with groups of compound standard names be represented by compound types?

Drawbacks with Compound Types

- Member fields have type and name, but are *not* netCDF variables
- Can't directly assign attributes to compound type members
  - New proposed convention solves this problem, but requires new user-defined type for each attribute
- Compound type not as useful for Fortran developers, member values must be accessed individually

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Example Convention for Member Attributes

```
types:
  compound wind_vector_t {
    float eastward ;
    float northward ;
    }
  compound wv_units_t {
    string eastward ;
    string northward ;
    }
dimensions:
    station = 5;
variables:
    wind_vector_t wind(station) ;
       wv_units_t wind:units = {"m/s", "m/s"} ;
       wind_vector_t wind:_FillValue = {-9999, -9999} ;
data:
    wind = {1, -2.5}, {-1, 2}, {20, 10}, ... ;
```

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Example Use of Enumerations

Named flag values for improving self-description:

```
types:
  byte enum cloud_t {
     Clear = 0, Cumulonimbus = 1, Stratus = 2,
     Stratocumulus = 3, Cumulus = 4, Altostratus = 5,
     Nimbostratus = 6, Altocumulus = 7, Missing = 127
     };
dimensions:
     time = unlimited;
variables:
     cloud_t primary_cloud(time);
        cloud_t primary_cloud:_FillValue = Missing;
data:
     primary_cloud = Clear, Stratus, Cumulus, Missing, …;
```

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Potential Uses for Enumerations

- Alternative for using strings with `flag_values` and `flag_meanings` attributes for quantities such as `soil_type`, `cloud_type`, ...
- Improving self-description while keeping data compact
- CF Conventions issues:
  - standardize on enum type definitions and enumeration symbols?
  - include enum symbol in standard name table?
  - standardize way to store descriptive string for each enumeration symbol?

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Example Use of Variable-Length Types

In situ observations:

```
types:
  compound obs_t {                // type for a single observation
    float pressure ;
    float temperature ;
    float salinity ;
  }
  obs_t some_obs_t(*) ;           // type for some observations
  compound profile_t {            // type for a single profile
    float latitude ;
    float longitude ;
    int time ;
    some_obs_t obs ;
  }
  profile_t some_profiles_t(*) ; // type for some profiles
  compound track_t {              // type for a single track
    string id ;
    string description ;
    some_profiles_t profiles;
  }
dimensions:
  tracks = 42;
variables:
  track_t cruise(tracks); // this cruise has 42 tracks
```

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Potential Uses for Variable-Length Type

- Ragged arrays
- In situ observational data (profiles, soundings, time series)

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Notes on netCDF-4 Variable-Length Types

- Variable length value must be accessed all at once (e.g. whole row of a ragged array)
- Any base type may be used (including compound types and other variable-length types)
- No associated shared dimension, unlike multiple unlimited dimensions
- Due to atomic access, using large base types may not be practical

Recommendations and Best Practices …

NetCDF Data Models and File Formats

Data providers writing new netCDF data have two obvious alternatives:

1. Use netCDF-3: classic data model and classic format

2. Use richer netCDF-4 data model and netCDF-4 format

and a third less obvious choice:

3. Use classic data model with the netCDF-4 format

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Third Choice: "Classic model" netCDF-4

- Psuedo format supported by netCDF-4 library with file creation flag
- Ensures data can be read by netCDF-3 software (relinked to netCDF-4 library)
- Compatible with current conventions
- Writers get performance benefits of new format
- Readers can
  - access compressed or chunked variables transparently
  - get performance benefits of reader-makes-right
  - use HDF5 tools on files

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NetCDF-4 Format and Data Model Benefits

HDF5-based format provides:

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New data model provides:

- Groups for nested scopes
- User-defined enumeration types
- User-defined compound types
- User-defined variable-length types
- Multiple unlimited dimensions
- String type
- Additional numeric types

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Why Not Make Use of NetCDF-4 Data Model Now?

- C-based netCDF-4 software still only in beta release (depending on HDF5 1.8 release)
- Few netCDF utilities or applications adapted to full netCDF-4 model yet
- Development of useful conventions will take experience, time
- Significant performance improvements available now, *without* netCDF-4 data model
  - using classic model with netCDF-4 format

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When to Use NetCDF-4 Data Model

- On “greenfield projects” (lacking legacy issues or constraints of prior work)
- If non-classic primitive types needed
  - 64-bit integers for statistical applications
  - unsigned bytes, shorts, or ints for wider range
  - real strings instead of fixed-length char arrays
- If making data self-descriptive requires new user-defined types
  - compound
  - variable-length
  - enumerations
  - nested combinations of types
- If multiple unlimited dimensions needed
- If groups needed for organizing data in hierarchical name scopes

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Recommendations for Data Providers

- Continue using classic data model and format, if suitable
- Evaluate practicality and benefits of classic model with netCDF-4 format
- Test and explore uses of extended netCDF-4 data model features
- Help evolve netCDF-4 conventions and Best Practices based on experience with what works

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Best Practices: Where to Go From Here

- We're updating current netCDF-3 Best Practices document before Workshop in July
- New "Developing Conventions for NetCDF-4" document is under development
- Benchmarks may help with guidance on compression, chunking parameters, use of compound types
- We depend on community experience for distillation into new Best Practices

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Adoption of NetCDF-4: A Three-Stage Chicken and Egg Problem

- Data providers
  - Won't be first to use features not supported by applications or standardized by conventions

- Application developers
  - Won't expend effort needed to support features not used by data providers and not standardized as published conventions

- Convention creators
  - Likely to wait until data providers identify needs for new conventions
  - Must consider issues application developers will confront to support new conventions

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Thanks!

Questions?