Report on the Workshop: Community Standards for Unstructured Grids

Held on October 16-17, 2006
Boulder, CO

By:

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Table of Contents

1. Executive Summary

NOAA and UCAR's Unidata Program sponsored a workshop to develop Community Standards for Unstructured Grids on October 16 and 17, 2006 in Boulder, Colorado. The goal of the workshop was to agree upon a provisional profile (i.e. metadata standards) for unstructured grid data that is stored in a netCDF format. This will be determined based upon an evaluation of the existing candidate profiles and issues that were identified at the workshop. Topics reviewed at the workshop consisted of unstructured metadata standards in use today, metadata standards in the IOOS context, CF conventions, XMDF data specification, and interoperability with users and processing applications. Breakout sessions focused on developing a common vision of needs and capability of unstructured grid models, and developing a core of conventions that can be regarded as a community starting point. The discussions begun at the workshop will be continued through an open, community moderated web site, which will result in a well-tested and widely-accepted standard for publication. The unstructured ocean model community should define a data model (in the language of OPeNDAP) and ensure the mapping of that model onto netCDF3 and HDF5 is functional.

2. Workshop Agenda

Sunday Evening, October 15

Reception starting at 6:30 pm at the Boulder Courtyard Marriott Hotel.

Monday, October 16

9:00 Welcome: Sandra Petrie (Unidata)

9:10 Introduction: Frank Aikman (NOAA/CSDL) and around the room

9:20 Overview of Workshop Goals and Unstructured Metadata Standards in Use Today: Straw man Example: Tom Gross (NOAA/CSDL)

9:40 Metadata standards in the IOOS Context: Steve Hankin (NOAA/PMEL and IOOS/DMAC)

10:10 Break

10:30 Important Aspects of the CF Conventions and Unidata Common Data Model: John Caron and Russ Rew (UCAR Unidata)

11:00 Breakout Session 1:
Morning Theme: Developing a Common Vision of Needs

Breakout sessions will discuss the extent of the vision of standards for irregular grids. What uses will a mesh standard have? How will it enhance the utility of ocean models to meet societal needs? How will visualization and web-services be improved by adoption of grid standards? How far a field from hydrodynamic modeling should we venture? Can a single system of hierarchical descriptions be devised to contain all of our needs? Where are the possible pitfalls and unsurpassable obstacles to this approach?

12:30 Lunch (provided)

1:30 Grids, Meshes and Mosaics: V. Balaji (NOAA/GFDL)

1:50 XMDF Data Specification and API in Support of Structured and Unstructured Data: Robert Wallace (USACE, ERDC-CHL-MS) and Alan Zundel (BYU)

2:10 Breakout Session 2:
Afternoon Theme: Grids in Great Detail

Breakout sessions will explore the complexities which must be included in an advanced grid spec. An emphasis should be placed on anticipating future needs and capabilities which exceed our present ability to work with and visualize model results. What requirements guided the development of existing irregular mesh models?

4:30 General Discussion and Recap of the Day

Tuesday, October 17

9:00 Plenary: Compare concrete results of breakouts and evening brainstorms

9:20 Users Often Need More Information About the Model Than You Think They Do: CJ Beegle-Krause and Chris Barker (NOAA/HAZMAT)

9:40 The importance of the API: some lessons from CF conventions for structured grids: Rich Signell (USGS) and CGNS: Thomas Hauser (USU)

10:00 Break

10:15 Breakout Session 3:
Morning theme: A core of conventions that can be regarded as a community starting point

Discussions will center on what core conventions can be adopted to start the process of integrating irregular mesh standards into modeling work. How will the more complex attributes of other grids be integrated into future specifications? Can an initial subset be described which is useful and agreed upon? What organizational structures will be needed to assure the adoption and future development of the standards?

12:00 Lunch (provided)

1:00 General Discussion

1:30 Breakout Session 4:
Afternoon Theme: What's left? What's the next step?

4:30 Reports from breakout groups: Action to be taken, next steps

3. Abstracts for Invited Talks

Tom Gross
Overview of Workshop Goals and Unstructured Metadata Standards in Use Today: Straw Man Example

This workshop is convened to discuss the development of standards for output products of irregular grid hydrodynamic models. These models are clearly a very important development in ocean science and are already in use by environmental managers and emergency response and planning management. The acceptance and support of these techniques will depend upon a usable interface between the modeling community and the 3rd party users of the model results. Many systems exist to work with simple, logically rectangular gridded models. The development of systems to work with triangulated meshes will require a community effort to provide a workable, reproducible, community supported irregular grid description. We believe that this is technically possible, and probably not very difficult. But it does require community buy-in for standards to be adopted and actually used. Community standards can provide non-altruistic benefits to model developers. If well designed then these descriptions can be the foundation of modeling tools which can be shared and will help the pace of development of irregular grid modeling methods.

We have a small collection of grid specifications for a few of the most popular irregular grid hydrodynamic models. A straw man "CDL" of these files will be posted and discussed. The possible uses of the data model will be described. The straw man is meant to be a starting point for the breakout session discussions of the details, exceptions and solutions for describing the greatest super-set of irregular griding methods.

This workshop will discuss the needs of the modelers and the 3rd party users of the models. Based on these needs we will build a description of an irregular grid data structure. Tangible examples will be devised for several existing modeling systems. Finally, we expect to propose to the CF Conventions for NetCDF a description of irregular meshes to be used by NetCDF output files. Other technologies will also be addressed, such as HDF5, Java API's etc. Steve Hankin - Metadata Standards in the IOOS Context

This workshop is sponsored through funding to develop a US Integrated Ocean Observing System (IOOS). This fact illustrates the degree to which coastal ocean modeling is a maturing field. Coastal ocean models are increasingly viewed as a primary tool for addressing day-to-day societal needs in areas such as mitigation of natural disasters; ecosystem and coastal resource management; public health; search and rescue; climate change impacts; navigation and homeland security. Addressing these "operational" needs today and in the near future requires community-wide adoption of standards for model output (among others) and an assurance that those standards will remain adequately stable.

The environment, in which modelers work, however, continues to evolve rapidly in many areas: numerical techniques, understanding of scientific processes, and the state of the art in information technology. The development of successful standards in areas of rapid technological advancement inevitably requires compromises that balance practical needs today, against anticipated needs in the future. This session will explore these issues and suggest some guidelines for the development of a successful standard.

John Caron and Russ Rew
Important Aspects of the CF Conventions and Unidata Common Data Model

The CF Conventions for netCDF metadata have proven extremely useful for describing climate and forecast model datasets stored in netCDF files. The Unidata Common Data Model (CDM) is an abstract data model for scientific datasets, combining the netCDF, HDF5, and OPeNDAP data models, and adds a coordinate system layer corresponding to that of CF. This talk will briefly summarize the coordinate system models of CF and the CDM, as background to possible extensions of CF for unstructured grids. We will also summarize the status and future developments of netCDF.

V. Balaji
Grids, Meshes and Mosaics

A grid-spec for irregular grids will need to fit into the larger context of other grid specifications in use by atmospheric climate models and the other world of regular gridded hydrodynamic models. A hierarchical grid spec is presented which may be used to contain complex grids which include staggered grids, sub-meshes, mosaics and other formulations necessary to efficient computing on cluster super computers. http://www.unidata.ucar.edu/events/2006GridWorkshop/balaji.pdf

Robert Wallace and Alan Zundel
XMDF Data Specification and API in Support of Structured and Unstructured Data

The XMDF API is probably the most complete API for Geophysical Fluid Dynamics. XMDF has a good users manual, both C and Fortran API, sits on top of HDF5. Uses include watershed, river, estuary and ocean models, and is evolving with HPC and GRID computing, OpenMI, ESMF and more. XMDF is built on HDF5 and includes both a data specification and an API to support structured and unstructured data. http://emrl.byu.edu/xmdf1/index.html

CJ Beegle-Kraus and Chris Barker
User's Often Need More Information About the Model Than You Think They Do

People that use model results, rather than run or develop models, often have different metadata needs than the modelers themselves. Potential uses are: emergency response, environmental effects, ecosystem modeling, and boundary conditions for other models. Key elements: The users are likely to need (1) model output values at arbitrary (x,y,z,t) locations in time and space, and (2) a great deal of knowledge about the grid, boundaries, and model domain.

<u>Rich Signell and Thomas Hauser</u>
<u>The importance of the API: some lessons from CF conventions for structured grid and CGNS</u>

The CF conventions seek to represent increasingly complex data relationships and grid structures. An Application Programming Interface, API, is a set of programs, subroutines and data structures which interface between the conventions and their actual use. An API is necessary to take advantage of the metadata conventions and allows generalization of application tools well beyond the one or two models originally targeted by the programmers.

A well conceived and supported API will avoid recoding the same logic and formula into each client application. NetCDF-Java is an API that gives access to many higher level CF operations for structured grids, such as returning coordinates for requested variables and computing vertical positions on-the-fly from stretched coordinate models. Examples will be shown using the NetCDF Java API in a stand-alone java client (IDV) and in a java-enabled analysis and visualization environment (Matlab).

How the API is designed and implemented can play a large role in how easy it is to develop clients and how efficiently and effectively those clients work. We need to discuss the relationship between the API, clients, and conventions as we formulate a strategy for interoperability with unstructured mesh data.

4. Synthesis of Breakout Sessions 1-3

Breakout sessions provided the bulk of the workshop. For the first three, participants were divided into three multi-interest groups to tackle similar issues in small groups. The final session held the group together to plot the way forward. These notes are organized with a short summary below, then the questions posed to each breakout, and, finally, notes coalesced from all the breakout groups.

The first three Breakout Session titles were:

Developing a Common Vision of Needs
Grids in Great Detail
Core of Conventions that can be Viewed as a Community Starting Point

The summary notes have the following headers:

Benefits of this standard
Requirements of a Standard – General Information
Vocabulary
Types of Models
The Way Forward

Where we began the meeting:

The community standards process is like herding cats, but much more worthwhile. A standard would help to separate science from data storage and from interpolation functions. Every modeler has their own file format and is inflexible / passionate about its use. The format most commonly uses ASCII or proprietary binary. Even if NetCDF is used for output files, these may be non-standard. Each model is unique; modelers working on a particular model or implementation are not generally interested in format.

Where we ended up:

Unstructured ocean model community should define a data model (in the language of OPeNDAP) and ensure the mapping of that model onto netCDF3 and HDF5 is functional Therefore the resulting web service will be OPeNDAP. (Then map back to netCDF, XMDF, GCMS). This would be an OPeNDAP2 compatible common data model. – Consensus is this is a reasonable straw man.

<u>Breakout Session One: Developing a Common Vision of Needs</u>

Breakout One will discuss the extent of the vision of standards for irregular grids.

- What uses will a mesh standard have?
- How will it enhance the utility of ocean models to meet societal needs?
- How will visualization and web-services be improved by adoption of grid standards?
- How far a field from hydrodynamic modeling should we venture?
- Can a single system of hierarchical metadata be devised to contain all of our needs? (netCDF 3 context)
- Where are the possible pitfalls and unsurpassable obstacles to this approach?

Summary Question: What are the essential usage requirements for a standard?

Breakout Session Two: Grids in Great Detail

Breakout Two will consider some of the complexities that must be included in an advanced grid spec.

1. What requirements guided the development of existing irregular mesh models?
2. List the objects and hierarchical connectivity that will describe the grids.
3. An emphasis should be placed on anticipating future needs and capabilities that exceed our present ability to work with and visualize model results.
4. Do supported file formats affect aspects of the proposed data models?

Summary Question: Are we able to put forth a comprehensive list of the quantities and design specifications? What will that contain?

Breakout Session Three: Core of conventions that can be regarded as a community starting point

Breakout Three discussions will center on what core conventions can be adopted to start the process of integrating irregular mesh standards into modeling work.

1. Can an initial "minimal" metadata for simple irregular grids be described that is useful and agreed upon?
2. How will the more complex attributes of other grids be integrated into future specifications?
3. What organizational structures are needed to assure the adoption and future development of the standards?
4. Is there agreement on file formats to support?
5. Is there an expansion path?

Summary Question: Does our path to agree upon and build a specification seem clear?

Benefits of an Unstructured Grid Standard

- Modeler's life easier
    - Visualization easy
    - Validation more easy
    - People with a favorite analysis tool will be able to use it with different models
    - Models (e.g. ADCIRC) can have this type of output inherent rather than programmer working on implementation (e.g. Chesapeake) having to code
    - Machine interoperability seems to be inherent
- User's life easier
    - You can open provider's file and you can get the right answer for your needs without going back to the provider
    - Machine interoperability seems to be inherent
    - Model to model interoperability inherent
    - Server to client easier
    - Client applications (e.g. MatLab, IDV, NCL, GMT, Ferret) will natively understand these files and utilize as easily as rectangular gridded models
    - Methods
        - Recommendations on how best to do secondary applications (e.g. gradients)
        - Server side regridding that conserves mass and tracers
        - Integrals and derivatives conservative
        - Users could use to construct API to do interpolation
    - Comparisons between models easier
        - between model implementations (e.g. various Chesapeake Bay) is straightforward
        - modeler to modeler
        - client deciding between implementations,
        - modeler -> analyst-> decision support products
- Merging a common data model would be beneficial for
    - observational data
    - unstructured models
    - structured models
- Break the tie between arrays and netCDF

Requirements of a Standard – General Information

- User group
  - Programmers – they get the data formatting and transfer work done
  - Modelers – (developers, providers and users)
    - Data products
    - Secondary analysis tools
  - Emergency Response (e.g. USCG and NOAA Hazmat)
    - Trajectory and SAR applications are being developed in grid independent formulation in order to take advantage of more models and model implementations.
    - Over 200 SAR cases are amenable to being solved by a better forecast model – need access to those forecasts.
  - Research scientists that are not modelers
  - Application (visualization, analysis, decision support) developers
  - Data managers
- Requirements of a convention
  - Human Needs
    - Learning curve for people getting started: easy to learn API
    - Data-discovery (human and automated) is functional.
    - Needs to work for model input (forcing and initialization) files also, not just output. This could stream-line run set-up time.
    - Coupling models (interpolation onto courser or finer grid) important (e.g. coupling to atmosphere and terrestrial models)
    - Most common grids handled well for models where vertical and horizontal grids are separable.
    - Modelers need to provide information
      - Model version
      - Provenance (software that created this)
      - Algorithms/References to do interpolation (specify in the file) – libraries are short term - this needs to be part of the standard.
    - Platform independent (can compile on a Macintosh)
    - Backward compatibility
    - Works with Balaji spec. (e.g. domain decomposition, coupling)
    - Ease of adapting existing applications and creating new ones
    - Pre-existence of libraries
    - Physical units
    - Quantity (e.g. kg/kg)
  - Computing Needs
    - Need a conceptual API for unstructured grids (this was intuitive for rectangular grids with hyperslabs)
    - Parallel processing (CPSs dump their data, but modern techniques allow parallel I/O to single file).
    - Efficiency of read and write (I/O efficiency in model run vs. efficiency for users of data).

    - minimize I/O operations;
    - minimize communication between nodes;
    - clustering data to do this
  - Should at least be able to write a restart file and any run-time I/O file (customer output). Majority of users need much more information than what is in a restart file.
  - Multi-file aggregation (directed structure to guide user to other files)
  - Server side subsetting is key.
  - Shared dimensions are important.
  - CGNS groups are used to breaking models into zones.
  - File indexing: files get too large to have linear scanning
  - Network access
  - Security
- Grid Details
  - Scalar and vector calculus on the field – this is a variable rather than formulation need.
  - Covers polygonal to simple layered triangular grids
  - Overlap with other grid tiles in a mosaic
  - Topology
    - Segment information (boundary and interior)
    - Connectivity
    - Searching
      - Where is a particular node or cell?
      - What is the data related to a particular node or cell?
      - Given latitude, longitude and time, what cell is the point in? Or on a boundary segment? Or outside domain?
- Methods
  - Methods (e.g. interpolation) are not part of standards, but users need them immediately.
  - Gradient calculations are function of the model and user's application (user beware).
- File formats to support
  - NetCDF3 (use of unlimited dimension significantly affects efficiency; doesn't have groups, structures or user-defined types)
  - NetCDF4 (goal of merging data models with OPeNDAP)
  - XMDF (HDF5) (already handles unstructured vertical coordinate)
  - CGNS (HDF5)
  - Relational Databases
  - ASCII (?)
- Georeferencing is key for analysis (census and biological data is generally in georeferenced database). Georeferencing information required for each node:

        - lat, long or x,y with projection, WKT (idealized simulations may not have this)
        - horizontal datum
        - vertical datum
        - time conventions
    - Next version will (slowly) deal with
        - Unstructured tetrahedral grids
        - Arbitrary 3D grids
        - Adaptive grids (change over time).
        - Unstructured vertical dimension
        - NetCDF4 version should be compatible with CGNS, XMDF HDF5 format.
        - Extruded and fully unstructured grids
    - Will there be unstructured grid models as we know them in five years? The community is moving to finite volume methods.
- What is the relationship between OPeNDAP and the CF standards?
    - Ambiguities between CF and the OPeNDAP footprint need to be examined carefully. (notion of shared dimensions among variables).
    - The extension comes with leaving Euclidean (x,y,z,t) dimensions behind and going to something that takes advantage of the "unstructured" elements?
    - Nodes on corners, edges, centers of elements; super grids – new issues due to new grids
    - We are hoping that we can write XDMF and CGNS connections to OPeNDAP.
- Requirements of the standards process
    - Build on what we know now
    - Standards name committee
    - Committee to create the proposal
    - Get it done in 6 months, define the level 0 baseline, then let's start making files
    - 6 month time-line – means saying "No" or "Later" to many things.
    - 80:20 – Can we get 80% of the way there for 20% of the work. One needs to know what 100% is (e.g. all the models) before you know you've got 80%.

Vocabulary

Model processes
- Nesting (one model running another)
- Coupling (models sharing data, e.g. coupled atmosphere ocean models)
- Chaining (data from one model used in another, e.g. ocean model used in a trajectory model)

Mosaic of grids
Grids (vs. Mesh)
Volume
    Number of faces
    - Triangular layer
    - Pyramid
    - Finite volume

Cells (vs. Elements)
    - Defined by specified edges and nodal values with interpolation functions; different orders of interpolation will require more information.
    - FEM's have basis functions across elements; FDM's have stencils on which methods are defined.
    - Number of Segments (vs. Surfaces vs. Faces)
        - Triangle (3)
        - Polygonal (n>3)
    - Segment (vs. Edge) type
    - Boundary type
    - Centroid
    - Area
    - Volume

Nodes (vs. Vertex)
- Polygon boundary nodes (most common)
- Interior nodes that are used in interpolation
- Face center

Mask (types of elements)
Topology (connectedness)
- Boundaries require a list of nodes (many choices)

Basis Functions
Recommended interpolation schemes

Types of models

- Node centered FE model
  - horizontal
  - 2D FE
  - triangular
  - polygonal
- Face centered FE model
- Spectral element (usually interpolated onto regular grid)
- Need to know all the models to tell whether or not we have 80%
  - FVCOM
  - ELCIRC, UNTRIM (similar grid)
  - ADCIRC (are other FE models subsets of this grid?)
  - RMA
  - QUODDY

5. The Way Forward (80% of the way/model type/functionality for 20% of the effort)

Unstructured ocean model community should define a data model (in the language of OPeNDAP) and ensure the mapping of that model onto netCDF3 and HDF5 is functional. Therefore, the resulting web service will be OPeNDAP (then map back to netCDF, XMDF, GCMS). This would be an OPeNDAP2 compatible common data model. – *Consensus is this is a reasonable straw man.*

Goals for This Process

First draft standard in 6 months

- List of models that will function under conventions (e.g. ADCIRC, QUODDY, etc.)
- Map XMDF vocabulary into Unidata Common Data Model, then have each of our models to fit into the standard, have modelers explain their grid in the new vocabulary in order to help comparison. (Less than 10)
- Implementable in netCDF 3
- Be careful that the new developments in modeling and in netCDF4 and HDF can be incorporated into the standard.
- Be prepared to say “No.” or “Later”
- An emphasis should be placed on anticipating future needs and capabilities that exceed our present ability to work with and visualize model results.

Implementation Process

Level 1

- Easy visualization (e.g. NCL, Visit, MatLab).
- Network connection for subsetting (remote access)

Level 2

- Find an arbitrary point not on a node.
- Interpolation.
- Put this model into another model (one way “chaining”)
- Operational needs so people to meet some of the 7 societal goals.

Level 3

- Regridding.
- Modeler’s doing interesting things with someone else’s models (coupling -> two way)

Level 4

- A white (or peer reviewed) paper would be a publication that allowed the community to compare grids between models with a common vocabulary. (Structured and unstructured grids)

6. Results of Breakout Session 4: What's left? What's the next step?

Unstructured Grids Task Lists

Milestone 1: Unstructured Grid Communications Tools

1. Create the wiki pages on CF pages
2. Populate with files from the older site
3. Add full suite of example CDL's
4. Create area for free discussion of methods
5. Email the group about the wiki with instructions to join and participate

Milestone 2: Unstructured Grid Vocabulary

1. Make a partial list
2. Find Synonyms from other sources, XMDF, CGNS etc.
3. Vote on a restricted vocabulary
4. Register with the MMI to create translations
5. Vector and tensor naming issues

Milestone 3: Unstructured Grid Example Files

1. Survey the world of unstructured models and make a page of links
2. Output file examples from multiple hydrodynamic models
    1. Quoddy, Tom Gross UgCdlQuoddy?
    2. ADCIRC, Jesse Feyen, Rick Luettich
    3. FVCOM, David Stuebe
    4. UnTRIM, Mike Piasecki
    5. ELCIRC/SELFE, Bill Howe (sample SELFE datasets)
    6. HYCOM, Carlos Lozano (Ashwanth)
    7. ROMS, Rich Signell
    8. POM, Tal Ezar
    9. TIDE2D/3D, Roy Walters
    10. RiCOM, Roy Walters
    11. MikeFV DHI, Ole Petersen
    12. RMA, Alan Zundel
3. Input file examples for multiple graphics packages
    1. NCL, Dave Brown
    2. Visit LLNL, David Stuebe
    3. Ferret & LAS, Steve Hankin
    4. ArcGIS, Nazila
    5. IDV, Don Murray
    6. Matlab, Tom Gross, R Signell

Milestone 4: Unstructured Grid Data Model

1. Discussion group for development
2. List server for this group.
    1. V. Balaji, John Caron, Rob Wallace, Alan Zundel, Thomas Hauser, Dave Stuebe, Jason Chaffey
3. Develop Data Model Description in:
    1. UML
    2. OPeNDAP DDS
    3. NetCDF CDL

Milestone 5: Unstructured Grid Draft Standard

1. Based on Simple CDL (T.Gross's HYDRONetCDF)
2. Generalize CDL to include edge variables
3. Add standard names decided in Milestone 2: Vocabulary

Milestone 6: Unstructured Grid External Surveys

1. Survey of many existing Models
2. Investigate CGNS
3. Investigate XMDF

7. Workshop Attendees

2006 Community Standards for Unstructured Grids Workshop Attendees

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