



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



## UXarray: Extending Xarray for Enhanced Support of Unstructured Grids

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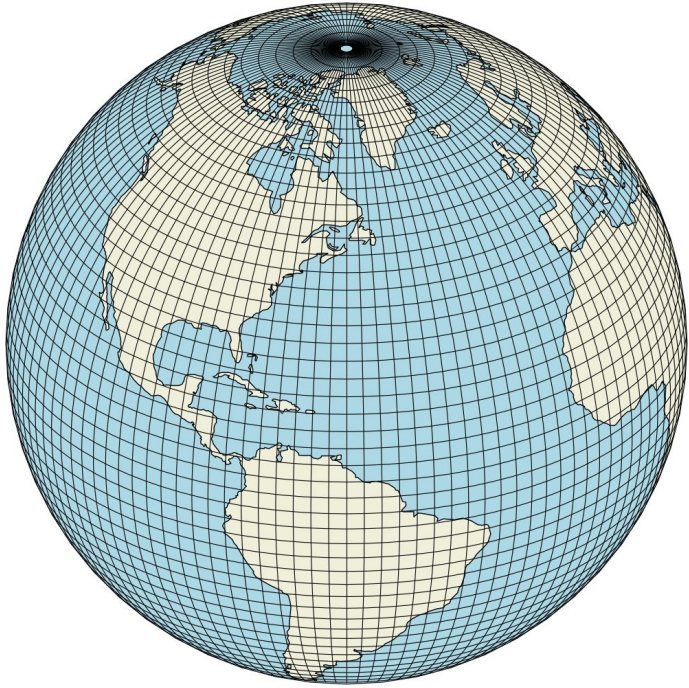
**(and many, many more!)**

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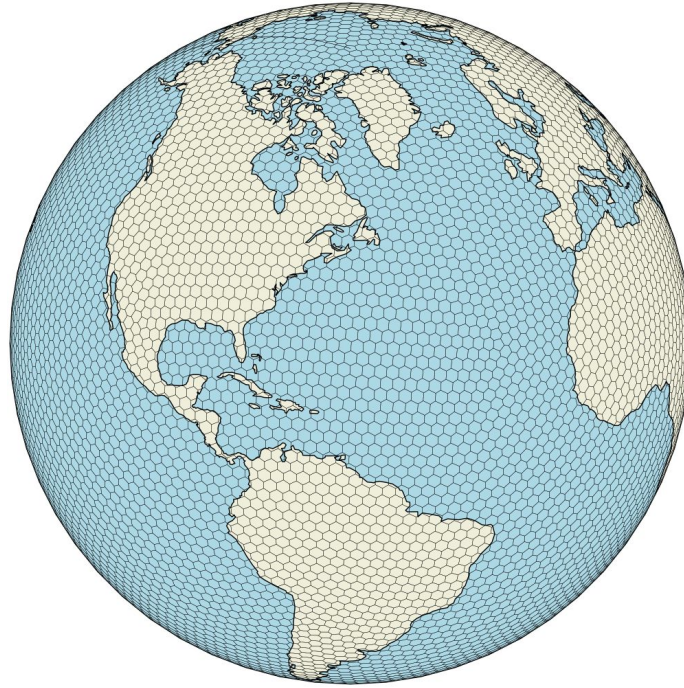
This material is based upon work supported by the National Science Foundation under Grants No.2126458 and 2126459

**May 2, 2025**

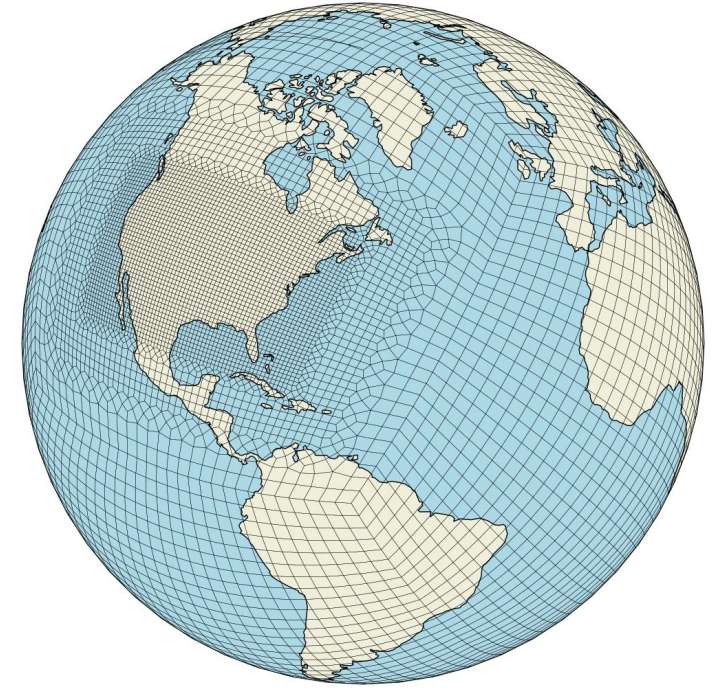
# Motivation: Arrival of kilometer-scale global models for weather and climate



Structured “lat-lon” grid



Voronoi grid



Variable resolution, cube-sphere

## Next generation, kilometer-scale climate and global weather models

After nearly two decades of development and evaluation, the climate and global weather modeling communities are transitioning from simple structured grids to more complex, but more scalable **unstructured grids** upon which governing equations of state are solved.

# Challenges

- ❖ No widely used convention for the storage of unstructured grid data
  - Though, UGRID is being adopted by some: <https://ugrid-conventions.github.io/ugrid-conventions/>
- ❖ Few analysis tools are capable of working directly with unstructured mesh data
  - Most, if not all, developed for a particular model's output only
  - Resampling to structured grids is common practice, but has myriad pitfalls
- ❖ Global storm resolving resolution models can generate LOTS of data
  - This further exacerbates problems with limited set of existing tools that operate directly on unstructured meshes
- ❖ Data operators that have trivial and efficient implementations with structured grids can become complex and computationally expensive with unstructured meshes
  - E.g. Efficiently finding the grid cell containing a point



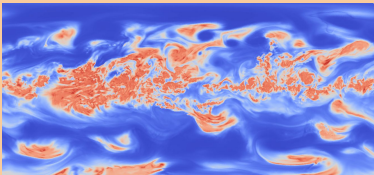
# Goals

1. Develop **extensible**, **scalable**, open source software for analysis and visualization of unstructured grid data from ESS models

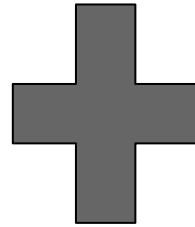
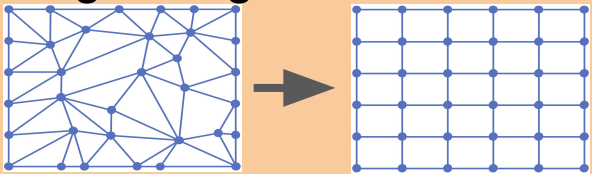
Computational operators

$$\mathcal{F}(x) \quad \frac{\partial x}{\partial y} \quad \mathcal{L}(x)$$

Plotting



Regridding



2. **Sustainable** and **community** owned

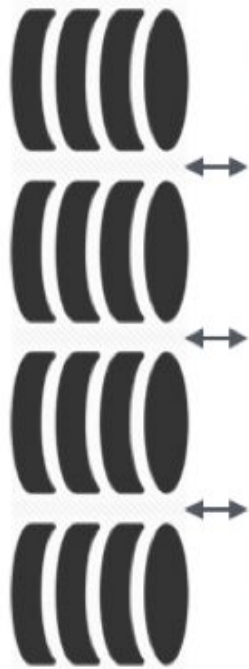


# Pangeo: A community platform for Big Data geoscience

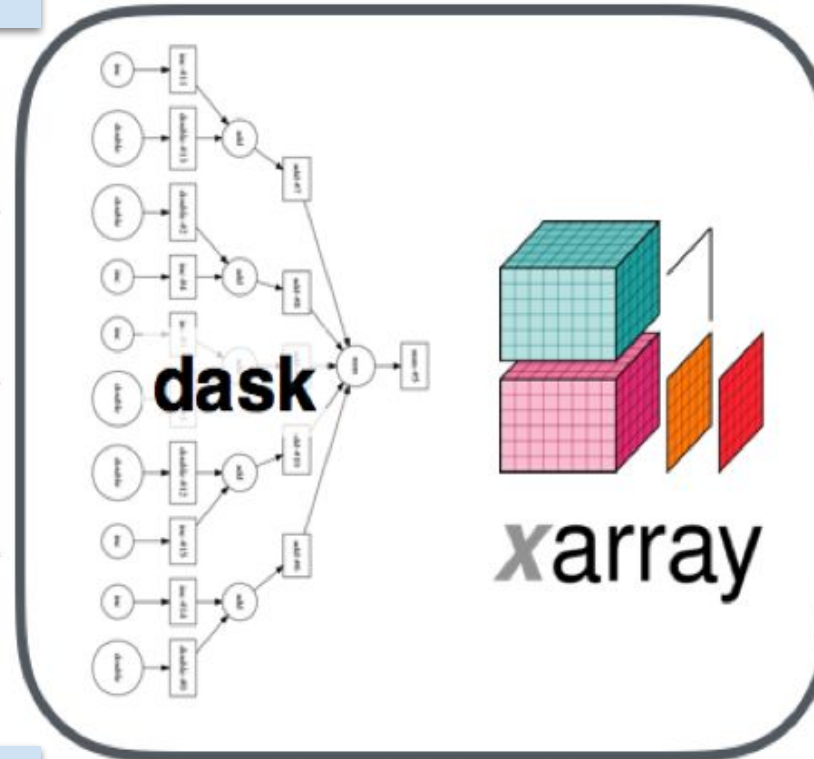


**Dask:** parallel compute for Python

storage nodes

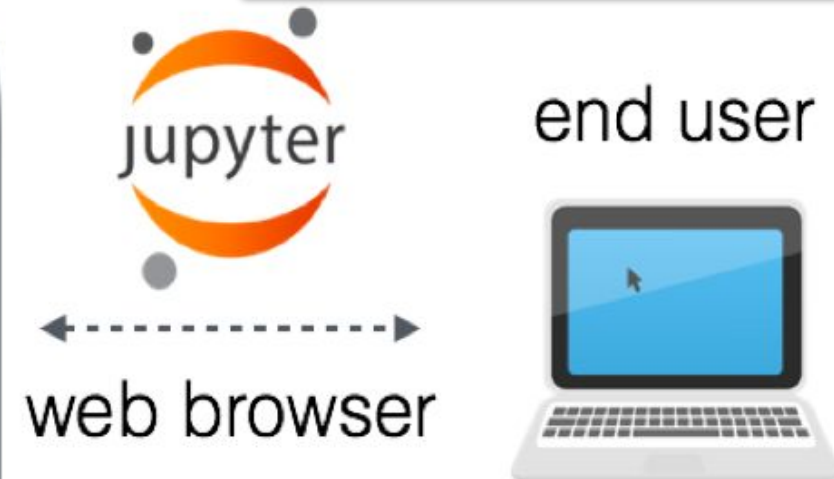


HPC / Cloud Compute



compute nodes

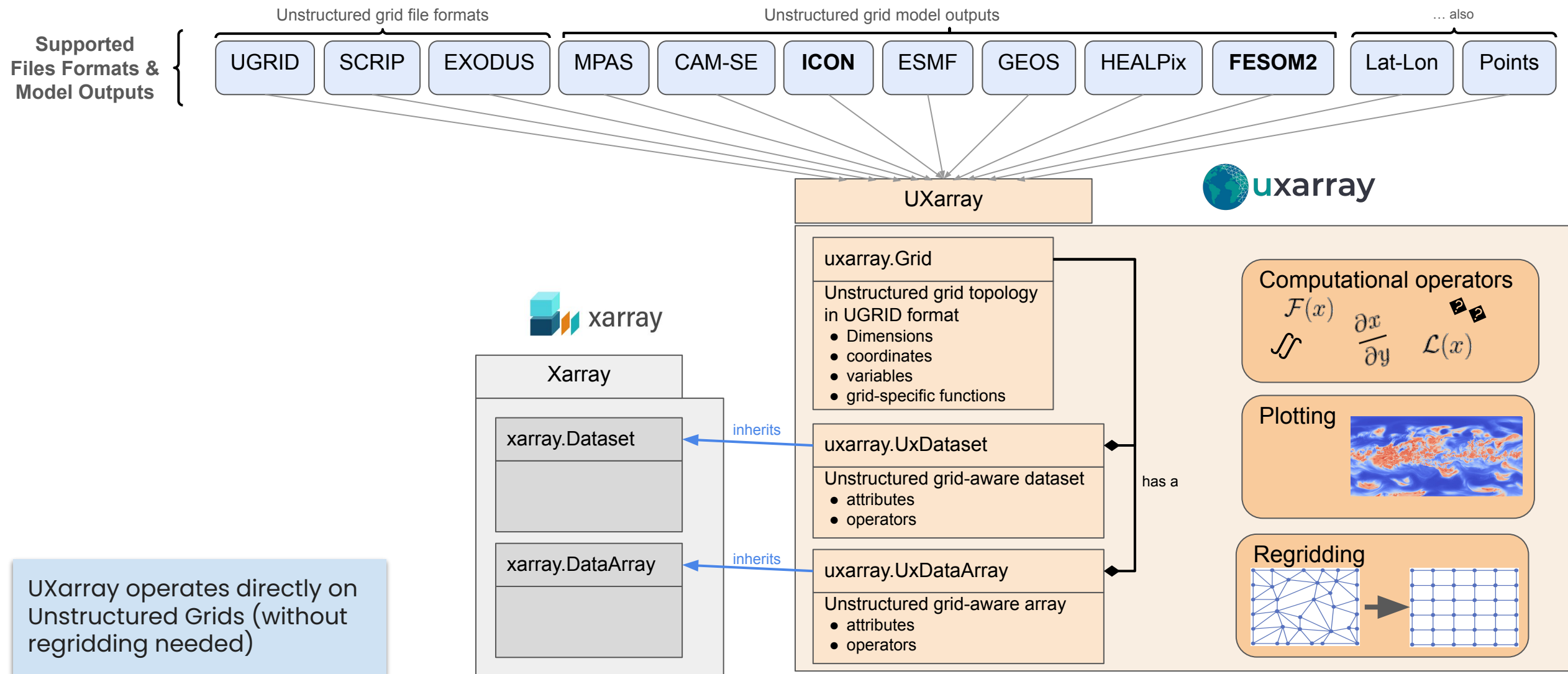
**JupyterHub:** platform agnostic, interactive access from a browser



**Xarray:** N-D labeled arrays with domain-agnostic functions for advanced analytics and visualization

Globally distributed,  
Analysis Ready, Cloud  
Optimized (**ARCO**) data

# UXarray: Xarray + unstructured grid awareness



# A sampling of UXarray's public class methods

```
# Open a dataset and analyze sea surface temperature
import uxarray as ux
uxds = ux.open_dataset(grid_file, data_file...)
grid = ux.open_grid(grid_file)
sst = uxds['sst']
```

## Operators inherited as is from Xarray (grid info not needed!)

```
sst.argmin()
sst.mean()
sst.where()
```

## Operators overridden from Xarray

```
sst.integrate()
sst.to_netcdf()
sst.plot()
```

## New operators added by UXarray

```
grid.plot()
sst.plot.points()
sst.gradient()
sst.topological_mean()
```

**Already using Xarray? UXarray should look pretty familiar!**

# Building the UXarray community

- **Everything on *public* GitHub**
- Open Source (Apache 2.0)
- **Built on Pangeo community AND Pangeo software stack**
- **Detailed contributors guide** + code of conduct
- Open discussion on all topics (GitHub Issues and Discussion forum)
  - Socialize major design decisions and roadmap
- **CI/CD infrastructure**
- Advocacy (conferences, discussion forums, events)
- A common programming language understood by scientists and software developers: **Python**
- **Lots of examples!**



UXarray Repository



# Current status - Functionality (as of release 2025.4.0)

## Supported model outputs / file formats:

- MPAS, CAM-SE, **ICON**, ESMF, GEOS, **FESOM2**, **HEALPix** models
- UGRID, SCRIP, EXODUS file formats
- Also structured grids and point-cloud data

## Grid manipulation

- Metadata inspection
- Subsetting (box, circle, NN)
- Remapping (NN, inverse distance weighted)
- Cross sections (Constant latitudes and longitudes)

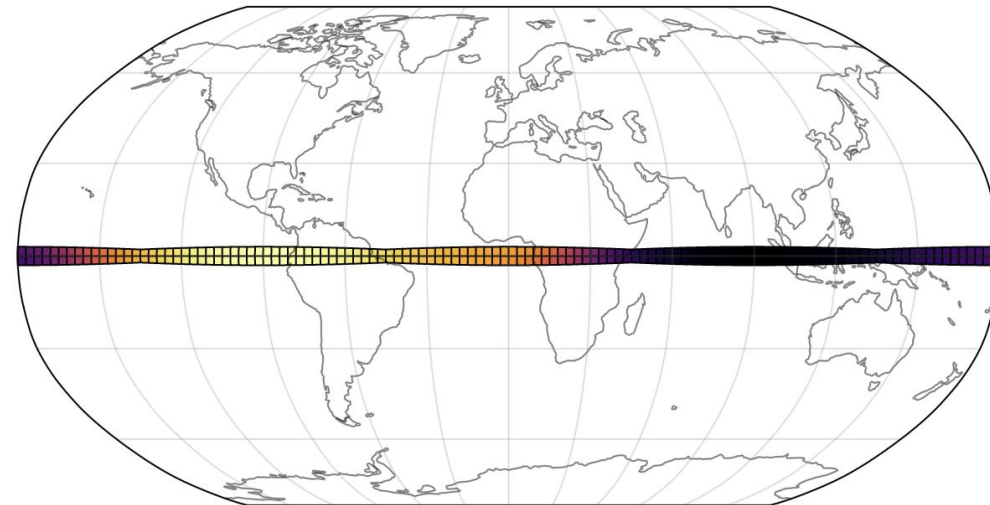
## Computational operators

- Non-conservative zonal means
- Global weighted averaging
- Integration
- Gradients
- Difference

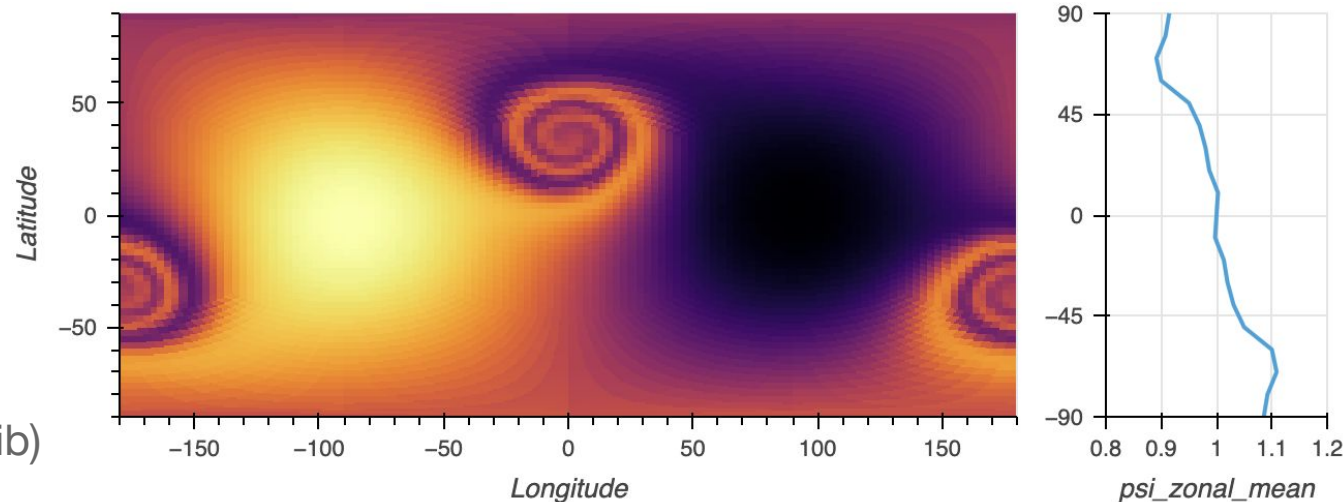
## Plotting

- Several functions for plotting mesh and data
- Interactive plots with Holoviz (Bokeh and Matplotlib)
- Outputs for native Matplotlib plots

### Cross-sections



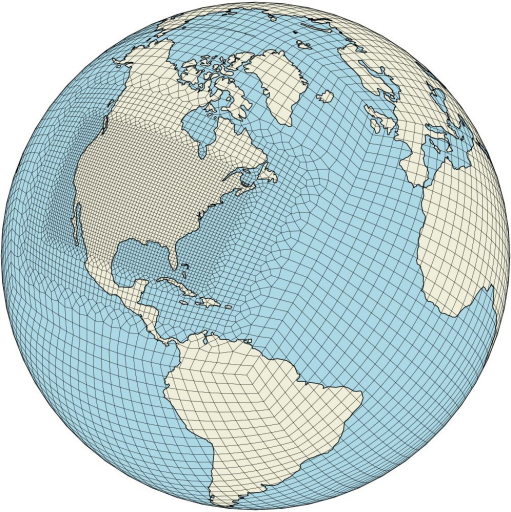
### Non-conservative zonal means



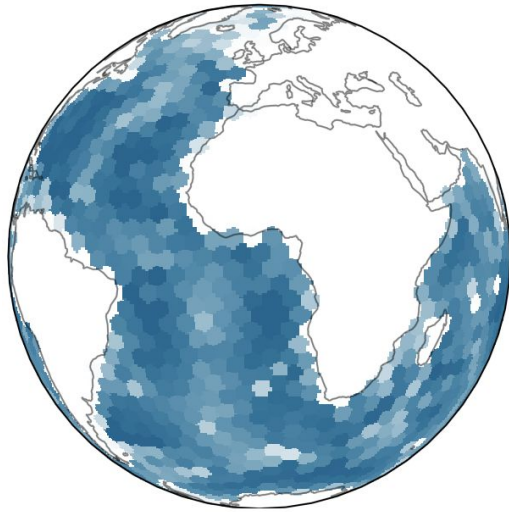


# Current status - Visualization

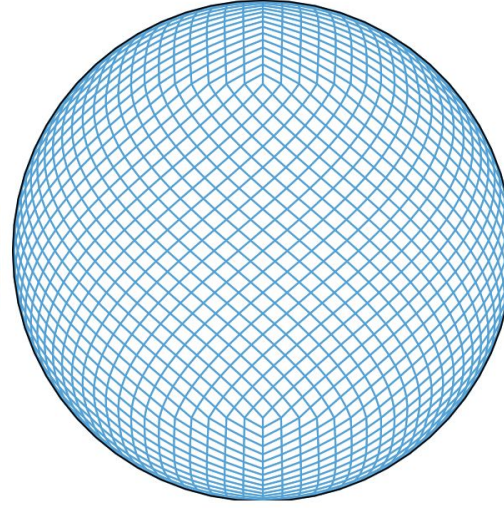
**CAM-SE**



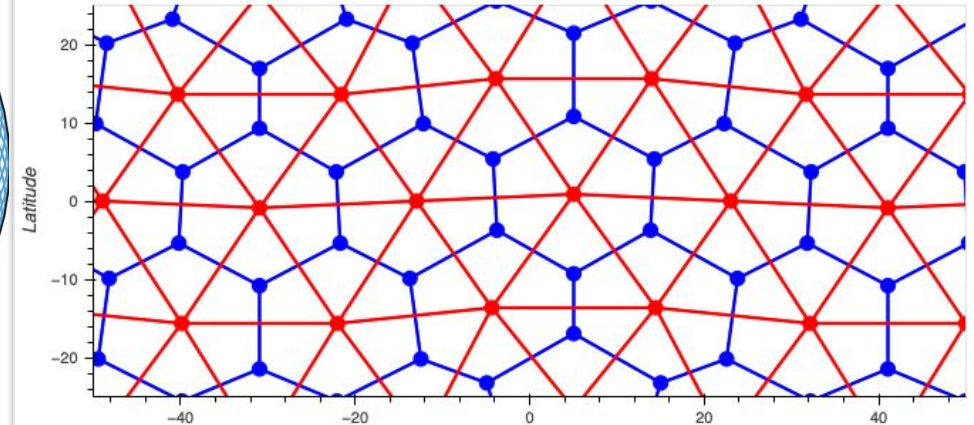
**MPAS**



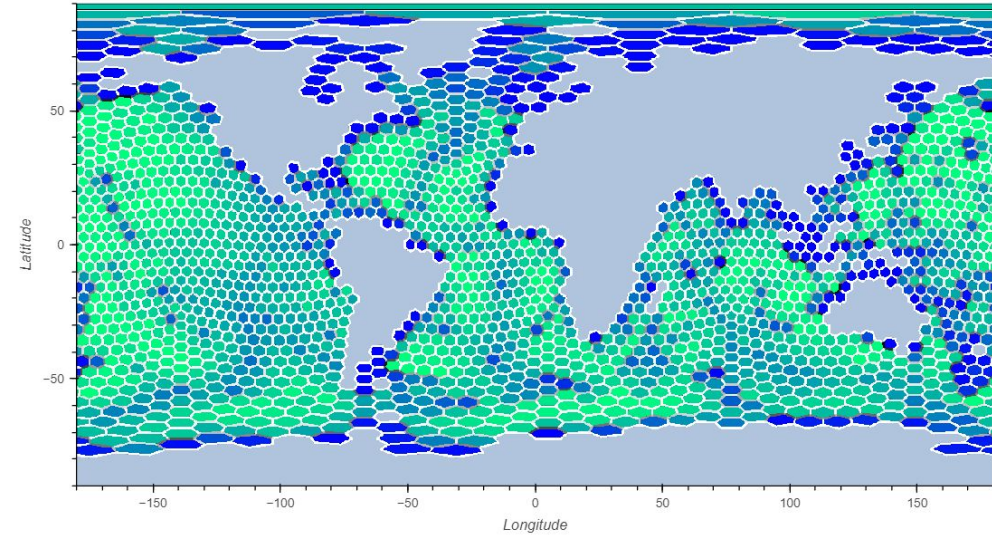
**HEALPix**



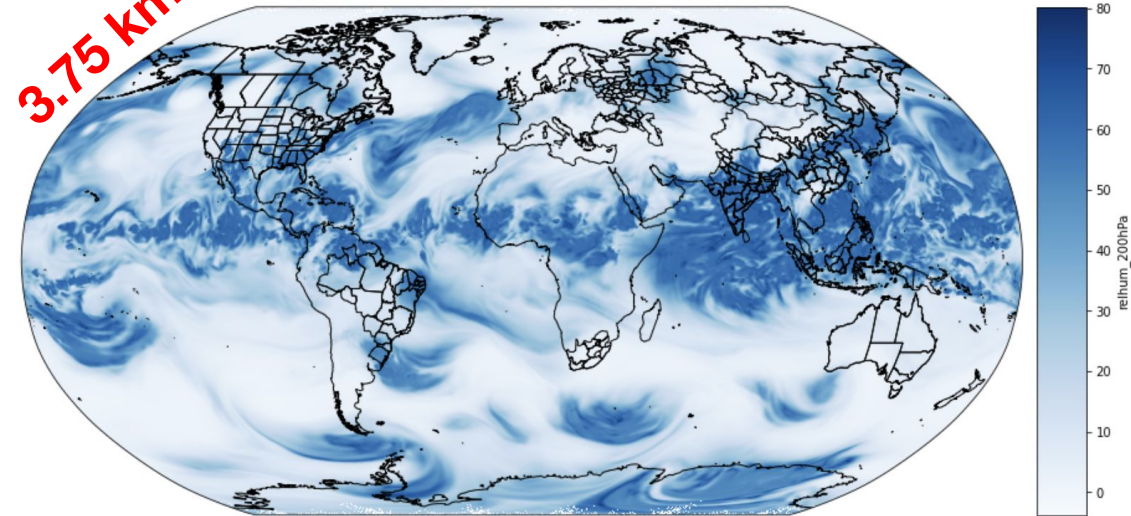
**MPAS Primal & Dual Mesh**



**Global Absolute Gradient**



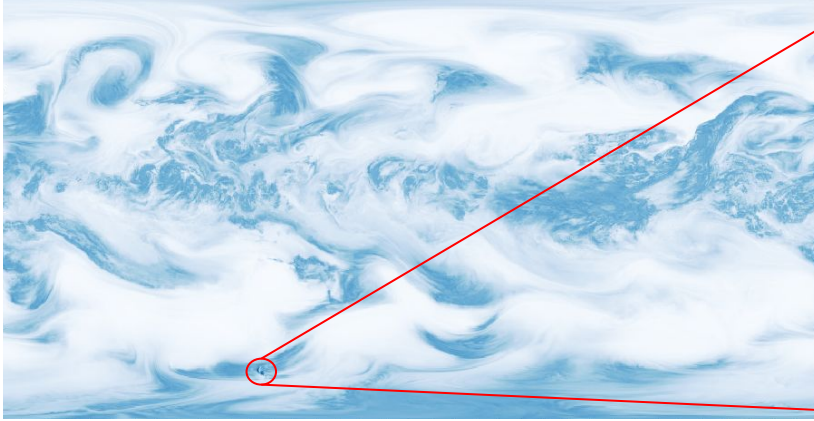
**3.75 km**



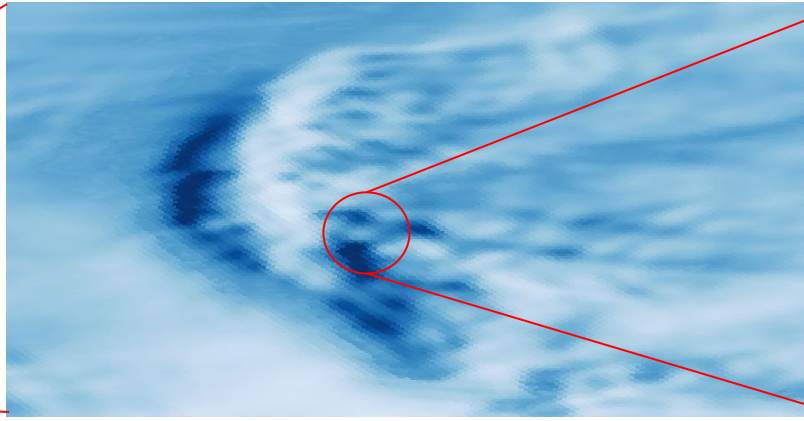


# Current status - Visualization

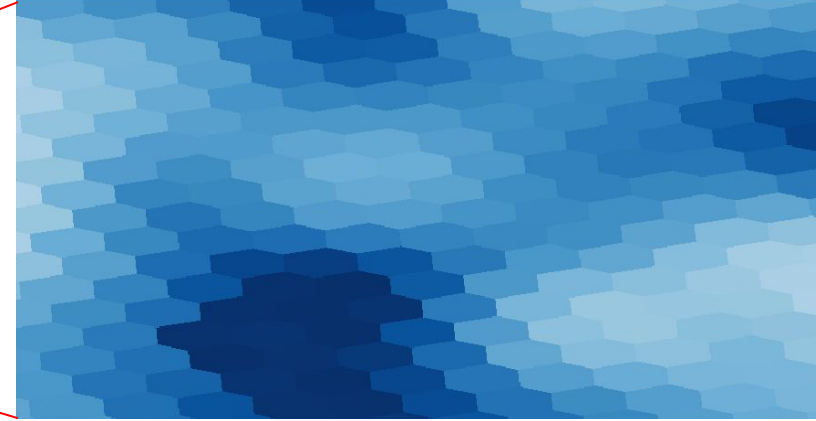
## High-Resolution Example: 3.75km MPAS Grid



**Global Polygon Raster**  
~42 million individual polygons



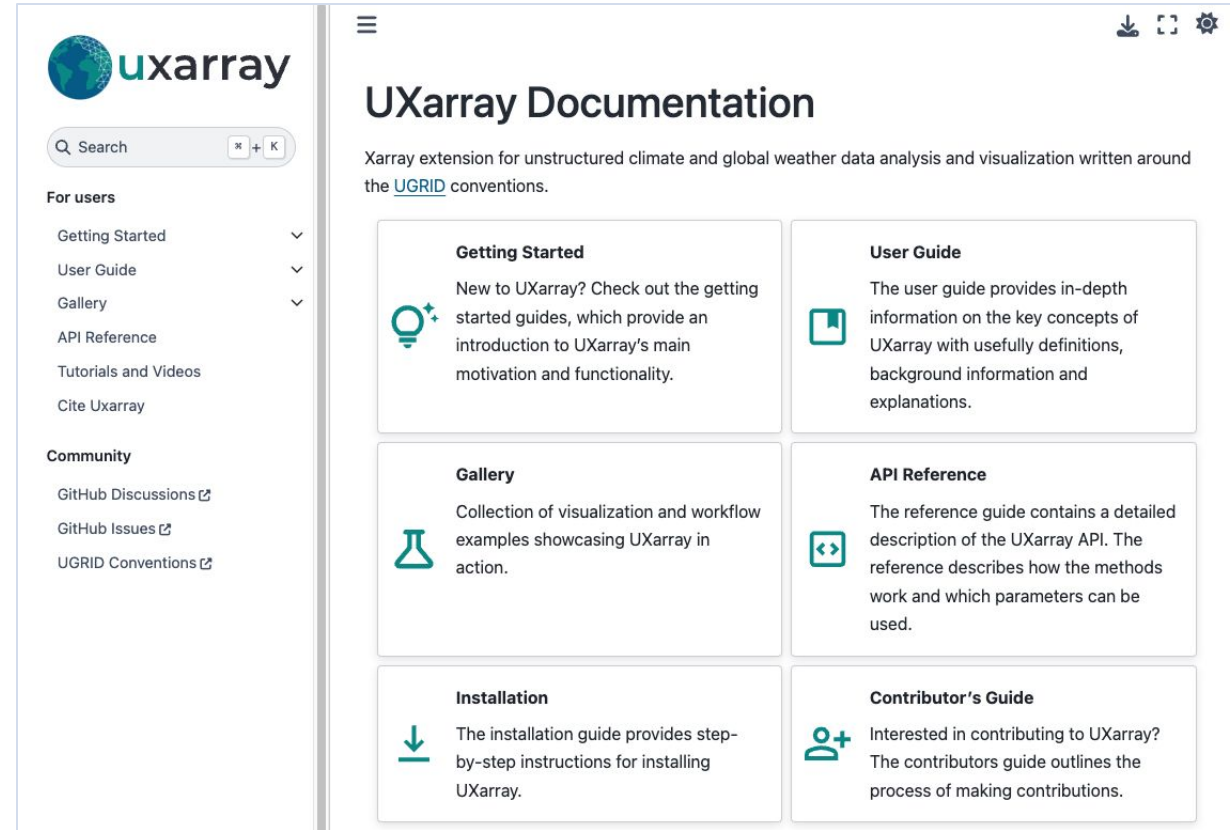
**Zoomed Raster**  
Begin to observe the underlying grid topology (hexagons)



**Further Zoomed Raster**  
After zooming far enough, the original hexagon grid becomes extremely clear

# Current status - Continuous delivery

- Public facing website
  - <https://uxarray.readthedocs.io/>
- **Comprehensive user documentation**
  - Getting started
  - User guide
  - Contributor's guide
  - Gallery
  - API reference
- **Monthly releases on conda and PyPi**
- Detailed examples (Jupyter Notebooks)



The screenshot shows the UXarray Documentation website. The sidebar on the left includes a search bar and navigation links for 'For users' (Getting Started, User Guide, Gallery, API Reference, Tutorials and Videos, Cite Uxarray) and 'Community' (GitHub Discussions, GitHub Issues, UGRID Conventions). The main content area is titled 'UXarray Documentation' and includes a description: 'Xarray extension for unstructured climate and global weather data analysis and visualization written around the UGRID conventions.' Below this are six cards: 'Getting Started' (New to UXarray? Check out the getting started guides...), 'User Guide' (The user guide provides in-depth information...), 'Gallery' (Collection of visualization and workflow examples...), 'API Reference' (The reference guide contains a detailed description...), 'Installation' (The installation guide provides step-by-step instructions...), and 'Contributor's Guide' (Interested in contributing to UXarray? The contributors guide outlines the process...).

## Xarray extension for unstructured climate and global weather data

CI passing CI Upstream passing pre-commit.ci passed codecov 86% docs passing benchmarked by asv  
tag v2025.03.0 conda-forge v2025.03.0 pypi v2025.3.0 license Apache-2.0 DOI 10.5281/zenodo.15007592



# Future work

Coming soon!

- Derivatives (advanced capabilities)
- Conservative zonal means
- Bilinear remapping

Longer term

- NSF CSSI proposal under review “Collaborative Research: Frameworks: UXarray - A sustainable tool to meet next generation earth system models’ analysis needs”
  - Appeal to other science domains (across the NSF GEO Directorate)
  - Become the go-to tool for working with unstructured grid earth sciences data
- New computational operators (div, curl, etc.)
- Plotting (Contours, vectors, etc.)
- More regridding as needed



Real time roadmap

## Lessons learned (from our scientific community)

- Git, GitHub and Python package management are barriers to many in the scientific community
- Jupyter Notebooks and JupyterHub are awesome!
- Dask is a technology for the 1% (at most)
- Socializing design decisions and feature requests can be super helpful
- Building a contributor community is really, really hard!

# The World Climate Research Programme Global km-scale Hackathon



**When: 12–17 May 2025**

**Where: 11 regional nodes worldwide**

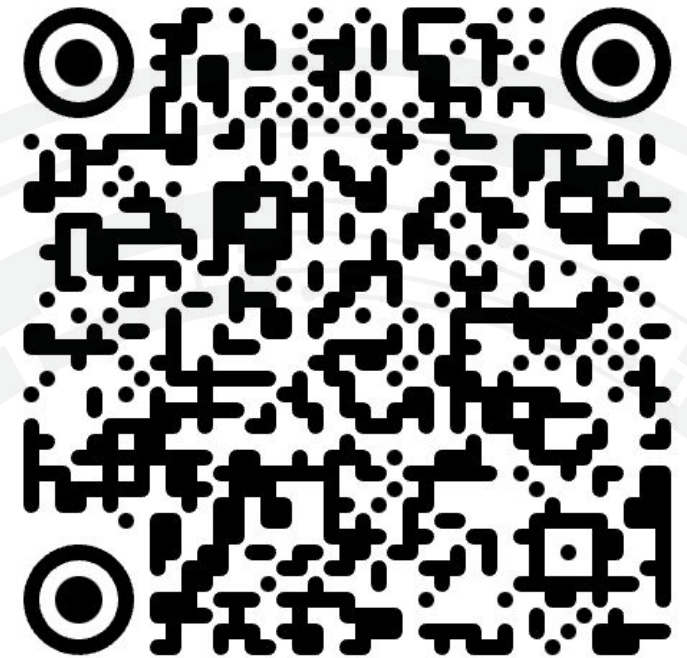
**Our partners:**



**WCRP**  
Digital Earth  
Lighthouse Activity



**For more  
information**



**Visit our website**

# Summary

UXarray is an **extensible**, **scalable**, open source Python package for analysis and visualization of unstructured grid data from ESS models.

Builds on top of a software ecosystem widely used by the ESS community; i.e. extends the **Xarray** package, supports **Dask** parallelization, documents with **Jupyter**, etc.

Supports a growing number of file formats & model outputs

Community driven and developed, with an increasing amount of global community contributions



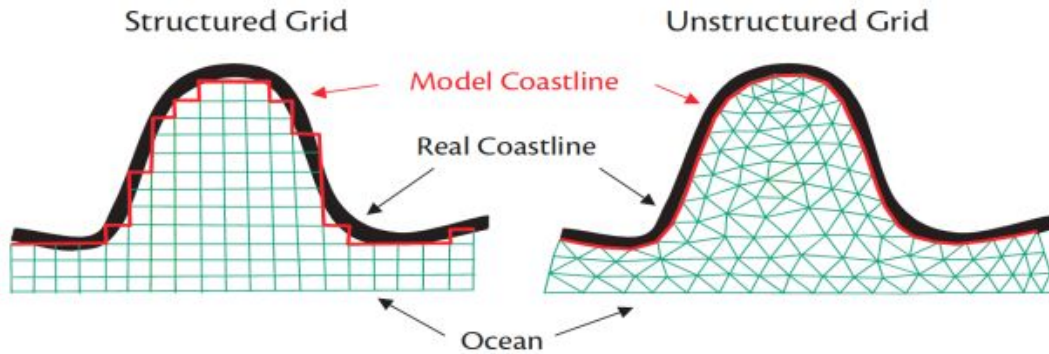
<https://uxarray.readthedocs.io>



# BACKUP

# Unstructured Grid Geometry

Adaptability to complex geometries

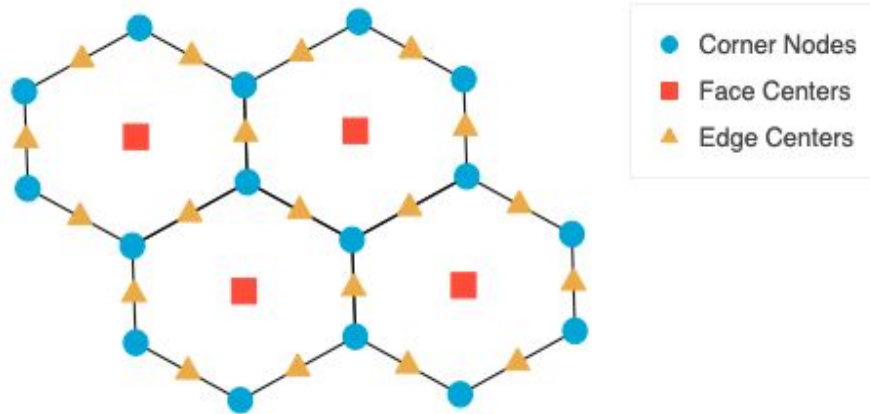


[Geometric adaptability \(example from FVCOM\)](#)

Local  
refinement



[Variable res. MPAS Voronoi grid](#)



Explicitly defined **connectivity** information for each geometric element; e.g.:

Connectivity	Dimension	Description
Face-Node	#Faces x #MaxPolygonNodes	Nodes' indices making up each face