yt-xarray, Facilitating Software Reuse Between Space and Earth Sciences

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Abstract

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CHAPTER

ONE

INTRODUCTION

Overview of the project.

Overview of the primary software pieces:

1.1 xarray

xarray: words: geo, NASA, cloud-native formats (zarr)

1.2 yt

more words

1.3 yt_xarray

more words

RECENT IMPROVEMENTS TO YT, YT_XARRAY

yt_xarray: yt api access:

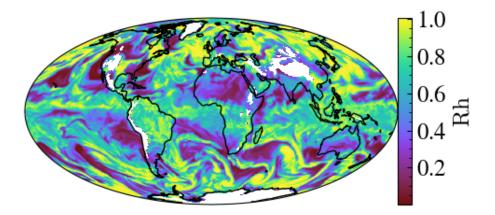
initial setup: silencing unrelated warnings and logs for brevity here.

load the data. data is local file, data is from the MERRA-2 reanalysis dataset (hosted at GES DISC, NASA EarthData)

```
import yt_xarray
import cartopy.feature as cfeature

dsx = yt_xarray.open_dataset("sample_nc/MERRA2_100.inst3_3d_asm_Np.19800120.nc4")

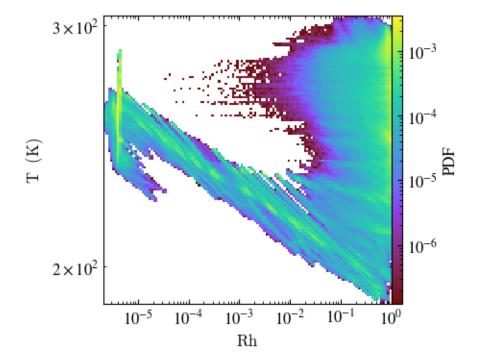
dsx0 = dsx.isel({'time':0})
slc = dsx0.yt.SlicePlot('altitude', 'RH', center=(800, 0.,0.))
slc.set_log('RH', False)
slc.render()
slc.plots['RH'].axes.add_feature(cfeature.COASTLINE)
slc.show()
```



```
import xarray as xr
import numpy as np
ones_da = xr.DataArray(np.ones(dsx0.RH.shape), dims=dsx0.RH.dims)
dsx0['ones_field'] = ones_da
```

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EMBEDDED TRANSFORMATIONS WITHIN YT XARRAY

In addition to providing methods for creating yt datasets that directly reference xarray datasets, ongoing development within yt_xarray PR #75) will provide a number of methods for building cartesian yt datasets with embedded transformations and interpolation of xarray datasets defined in non-cartesian coordinates. This approach provides a convenient way of utilizing yt methods that rely on cartesian geometries without having to pre-interpolate data, making reproducible workflows to, for example, generate 3D volume renderings much simpler to make.

The general workflow is

- 1. open the xarray dataset
- 2. define the transformation from the dataset's native coordinates to cartesian coordinates
- 3. define the method of interpolation
- 4. initialize the yt dataset
- 5. In pseudo-code, the above steps look like:

```
import yt_xarray
from yt_xarray.transformations import GeocentricCartesian, build_interpolated_
cartesian_ds

ds = yt_xarray.open_dataset(...) # or xr.open_dataset
gc = GeocentricCartesian(...)
ds_yt = build_interpolated_cartesian_ds(ds, gc, ...) # a cartesian yt dataset
```

Initially, build_interpolated_cartesian_ds only sets up the cartesian grid (or grids) that will be used to wrap the non-cartesian geometry and actual interpolation of the data onto the cartesian grid (or grids) is delayed until yt needs the data. During initialization of the yt dataset (build_interpolated_cartesian_ds, step 4 above), the user can specify parameters that control how the cartesian grid is built. For example, the following pseudo-code:

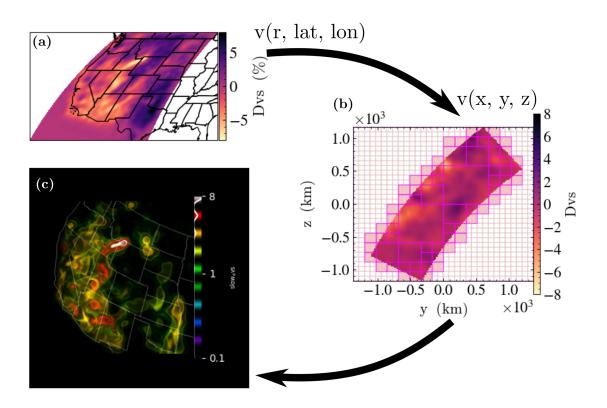
```
build_interpolated_cartesian_ds(
    ds,
    gc,
    grid_resolution=(16,16,16),
    refine_grid=True,
    refine_by=8,
    refine_min_grid_size=2,
    ...)
```

grid_resolution specifies the coarse grid resolution of 16 cells in each dimension. When refine_grid is True, yt_xarray will apply a recursive subdivision of the domain into a number of smaller grids: starting from the coarse grid, the domain is divided in half along each dimension and grid cells are filled with a binary image mask, where cell values are set to 1 if they fall within the bounds of the non-cartesian geometry. Division proceeds recursively, with empty grids being discarded, until the remaining grids satisfy an adjustable fill criteria (or the max number of iterations has been

reached). In addition to the recursive bisection, one may use an implementation of **CITATION** (berger and rigoutsos 1991, https://doi.org/10.1109/21.120081) by setting refinement method='signature filter'.

In the following, two examples with real datasets are described, with images from sequential stages of the above transformation workflow along with a final 3D volume rendering. The first example uses a seismic tomography model of the Earth's upper mantle beneath the Western U.S. **CITATION**, while the second uses a MERRA-2 netcdf file from **CITATION**.

3.1 Volume Rendering Workflow: Seismic Tomography



- (a) The data is initially loaded with xarray in native coordinates which in this case is internal geodetic coordinates (depth beneath the Earth's surface, latitude and longitude). From here, all the usual xarray methods apply: the image here is a slice at 100 km depth through shear wave speed anomalies (Dvs), generated in this case with yt_xarray's convenience wrapper of yt.SlicePlot (see previous section).
- (b) After defining the transformation from geodetic coordinates to cartesian coordinates, a wrapping cartesian grid is refined to generate a cartesian yt dataset. This cartesian dataset can be used with any yt method. A yt. SlicePlot with grid and cell annotations illustrates the refined grid structure: the squares outline in bold represent the edges of grids while fainter lines indicate grid cells. The starting grid here was 32x32x32 with a refinement factor of 8, resulting in a dense sampling where there is data in the underlying geometry. In constructing this plot, yt will access data only in the grids intersected by the desired cutting plane and grids are processed individually. This means that only a subset of the full dataset is interpolated on-demand, as needed by yt.
- (c) Once the cartesian yt dataset is available, methods in yt that rely on cartesian ray tracing are available to use. The image here is a 3D volume rendering of only the slow velocity anomalies (where Dvs is less than 0). The transfer function used here consists of a number of gaussian samples of the data spaced linearly between 0.1 and 8 percent and results in a clear signal of the Yellowstone hot spot track beneath northeast Idaho and northwest Wymoing, where high temperatures and partially molten rock decrease the shear wave speed

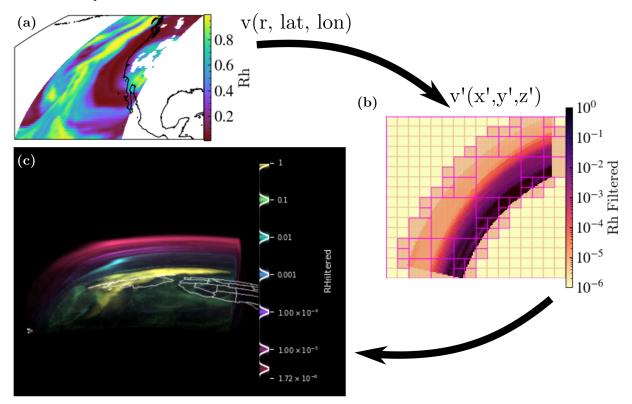
In pseudo, code the above steps are

The full code is available at code repository associated with these materials.

3.2 Volume Rendering Workflow: Atmospheric Geophysics, MERRA-2

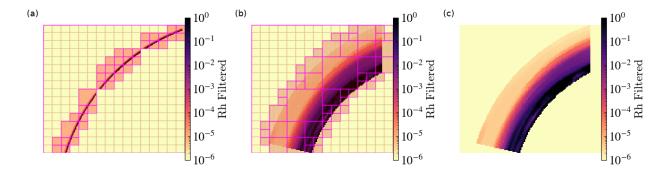
The second example demonstrates some of the difficulty of volume rendering with geophysical data. In addition to having to interpolate to cartesian coordinates, the vertical length scale present in data

MERRA-2 example



- (a) Data defined in (pressure level, latitude, longitude). Relative humidity
- (b) Transformation here: pressure level to height, apply a radial scale factor and then convert to "virtual" cartesian coordinates.
- (c) The volume rendering here caputres the coherence of the high relative humidity features in 3D. Also, missing data is a challenge for volume rendering: set to 0.0 and transfer function chosen to exclude those 0.0 values.

The following image further illustrates the difficulty of volume rendering with short relative radial length scales:



In panel (a), a cartesian grid is constructed from the raw data subsample, without applying any vertical exaggeration factor. Over the length scales required to capture features of interest (tens of degrees), the relative thickness of the atmosphere is difficult to resolve (the grid refinement actually breaks down and misses some points). Panels (b) and (c) demonstrate the same data with a radial scale factor of 20., resulting in a virtual cartesian grid that can reasonably resolve features within the atmosphere.

CHAPTER

FOUR

UTILIZING CLOUD NATIVE DATA FORMATS WITH YT_XARRAY

4.1 zarr via xr

xr backend allows zarr access: simple demo?

4.2 zarr with yt

zarr with yt paragraph or two

CHAPTER FIVE

SUMMARY

In summary

CHAPTER

SIX

TECHNICAL APPENDIX

notebook requirements, notes on use of development branches, etc.

6.1

development branches:

yt: need dev (until yt4.4, geoquiver) yt_xrarray: need PR branch

6.2 building this book

Recommended that you use pdflatex directive to build the pdf, which requires that you first install a texlive distribution, see

https://jupyterbook.org/en/stable/advanced/pdf.html

```
$ pyenv virtualenv 3.10.11 yt_NASA_SMD
$ pyenv activate yt_NASA_SMD
```

from top level

```
$ pip install -r requirements.txt
$ jupyter-book build yt_xr_2024/ --builder pdflatex
$ cp yt_xr_2024/_build/pdf/book.pdf ./yt_xr_2024.pdf
```

6.3 all the data